AB SCIEX 6500 Series of Instruments

System User Guide

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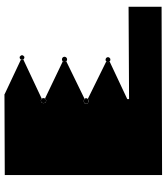

AB Sciex Pte. Ltd.
Blk 33, #04-06
Marsiling Ind Estate Road 3
Woodlands Central Indus. Estate
SINGAPORE 739256

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Operational Precautions and Limitations 1

This section contains general safety-related information and provides regulatory compliance information. It also describes potential hazards and associated warnings for the system, and the precautions that should be taken to minimize the hazards.

In addition to this section, refer to Hazards Symbols on page 17 for information on the symbols and conventions used in the laboratory environment, on the system, and in this documentation. Refer to the *Site Planning Guide* for site requirements, including AC mains supply, source exhaust, ventilation, compressed air, nitrogen, and roughing pump requirements.

General Safety Information

To prevent personal injury or system damage, read, understand, and obey all safety precautions, warnings in this document, and labels on the mass spectrometer. These labels are shown with international symbols. Failure to heed these warnings could result in serious injury.

This safety information is intended to supplement federal, state or provincial, and local environmental health and safety (EHS) regulations. The information provided covers system-related safety with regard to the operation of the mass spectrometer. It does not cover every safety procedure that should be practised. Ultimately, the user and the organization are responsible for compliance with federal, state or provincial, and local EHS regulations and for maintaining a safe laboratory environment.

For more information, refer to the appropriate laboratory reference material and standard operating procedures.

Regulatory Compliance

This system complies with the standards and regulations listed in this section. Applicable labels have been affixed to the system.

Australia and New Zealand

- **Electromagnetic Interference**—AS/NZ CISPR 11 (Class A)
- **Safety**—AS/NZ 61010-1

Canada

- **Electromagnetic Interference**—CAN/CSA CISPR11. This ISM device complies with Canadian ICES-001.
- **Safety**—CAN/CSA C22.2 No. 61010-1, and CAN/CSA C22.2 No. 61010-2-061

Europe

- **Electromagnetic Compatibility**—Electromagnetic Compatibility Directive 2004/108/EC, as implemented in these standards:
  - EN 55011 (Class A)
  - EN 61326-1
- **Safety**—Low Voltage Directives 2006/95/EC as implemented in these standards:
  - EN 61010-1
  - EN 61010-2-061
- **WEEE**—Waste, Electrical, and Electronic Equipment Directive 2002/96/EEC

United States

- **Electromagnetic Interference, FCC Part 15, Class A**—This equipment has been tested and found to comply with the limits for a Class A digital device, pursuant to Part 15 of the FCC (Federal Communications Commission) Compliance Rules.

  These limits are designed to provide reasonable protection against harmful interference when the equipment is operated in a commercial environment. This equipment generates, uses, and can radiate radio frequency energy and, if not installed and used in accordance with the operator's manual, can cause harmful interference to radio communications.

  Operation of this equipment in a residential area is likely to cause harmful interference in which case you will be required to correct the interference, at your own expense. Changes or modifications not expressly approved by the manufacturer could void your authority to operate the equipment.
- **Safety**—UL 61010-1, IEC 61010-2-061

International

- **Electromagnetic Compatibility**—IEC 61326-1, IEC CISPR 11 Class A
- **Safety**—IEC 61010-1, IEC 61010-2-061

For more information, refer to the Declaration of Conformity included with the system.

Electrical Precautions

AC Mains Supply

WARNING! Electrical Shock Hazard: Use only qualified personnel for the installation of all electrical supplies and fixtures, and make sure that all installations adhere to local regulations.

Caution: Potential System Damage: Do not unpack or connect any components. The Field Service Employee (FSE) will unpack, connect, and configure the system for the proper operating voltage.

For information on system electrical specifications, refer to the *Site Planning Guide*.

Protective Earth Conductor

The mains supply must include a correctly installed protective earth conductor that must be installed or checked by a qualified electrician before connecting the mass spectrometer. The mass spectrometer must be positioned to permit access to the mains supply connector to disconnect the device.

WARNING! Electrical Shock Hazard: Do not intentionally interrupt the protective earth conductor. Any interruption of the protective earth conductor is likely to make the installation dangerous.

Chemical Precautions

- Determine which chemicals may have been used in the system prior to service and regular maintenance. Refer to Safety Data Sheets for the health and safety precautions that must be followed with chemicals.
- Work in a well-ventilated area.
- Always wear assigned personal protective equipment, including powder-free nitrile gloves, safety glasses and a laboratory coat.
- Follow required electrical safe work practices.
- Avoid ignition sources when working with flammable materials, such as isopropanol, methanol, and other flammable solvents.

- Take care in the use and disposal of chemicals and comply with all local regulations to avoid potential risk of personal injury.
- Avoid skin contact with chemicals during cleaning, and wash hands after use.
- Comply with all local regulations for the storage, handling, and disposal of biohazard, toxic, or radioactive materials.

System Safe Fluids

The following fluids can safely be used with the system.

Caution: Potential System Damage: Do not use any other fluid until confirmation is received from AB SCIEX that it will not present a hazard. This is not an exhaustive list.

- Organic solvents
  - MS-grade acetonitrile; up to 100%
  - MS-grade methanol; up to 100%
  - Isopropanol; up to 100%
  - Tetrahydrofuran; up to 100%
  - Toluene and other aromatic solvents; up to 100%
  - Hexanes; up to 100%
  - HPLC-grade or higher water; up to 100%
- Buffers
  - Ammonium Acetate; less than 1%
  - Ammonium Formate; less than 1%
  - Phosphate; less than 1%
- Acids and Bases
  - Formic Acid; less than 1%
  - Acetic Acid; less than 1%
  - Phosphoric Acid; less than 1%
  - Trifluoroacetic Acid; (TFA) less than 1%
  - Heptafluorobutyric Acid; (HFBA) less than 1%
  - Ammonia/Ammonium Hydroxide; less than 1%
  - Trimethylamine; less than 1%
  - Triethylamine; less than 1%

Refer to Service and Maintenance Information on page 121 for information on safe cleaning solutions.

Ventilation Precautions

The venting of fumes and disposal of waste must be in accordance with all federal, state, provincial, and local health and safety regulations. Use the system indoors in a laboratory that complies with the environmental conditions recommended in the *Site Planning Guide* for the system.

The source exhaust system and roughing pump must be vented either to an external fume hood or to an external exhaust system as recommended in the *Site Planning Guide* for the system.

WARNING! Asphyxiation Hazard: Take care to vent exhaust gases properly. The vent tubing must be secured with clamps. The use of mass spectrometers without adequate ventilation to outside air might constitute a health hazard. In addition, certain procedures required during the operation of the mass spectrometer might cause gases to be discharged into the exhaust stream. Under these conditions, inadequate ventilation might result in serious injury.

WARNING! Toxic Chemical Hazard, Biohazard, Radiation Hazard: Make sure that the mass spectrometer is connected to the local exhaust system and ducted to control hazardous emissions. The system should only be used in a well-ventilated laboratory environment in compliance with local regulations and with appropriate air exchange for the work performed. Some jurisdictions recommend 4 to 12 air changes per hour in laboratories.

WARNING! Potential Toxic Chemical Hazard, Biohazard, Radiation Hazard: Do not operate the mass spectrometer if the source exhaust drain and roughing pump exhaust hoses are not properly connected to the laboratory ventilation system. Perform a regular check of the exhaust tubing to ensure that there are no leaks.

Environmental Precautions

Use qualified personnel for the installation of electrical mains, heating, ventilation, and plumbing supplies and fixtures. Make sure that all installations follow local bylaws and biohazard regulations. For more information about the required environmental conditions for the system, refer to the *Site Planning Guide*.

DANGER! Explosion Hazard: Do not operate the system in an environment containing explosive gases. The system is not designed for operation in an explosive environment.

WARNING! Asphyxiation Hazard: Take care to vent exhaust gases properly. The use of mass spectrometers without adequate ventilation to outside air might constitute a health hazard. In addition, certain procedures required during the operation of the mass spectrometer might cause gases to be discharged into the exhaust stream. Under these conditions, inadequate ventilation might result in serious injury.

WARNING! Toxic Chemical Hazard, Biohazard, Radiation Hazard: Make sure that the mass spectrometer system is connected to the local exhaust system and ducted to control hazardous emissions. Use the system only in a well-ventilated laboratory environment, in compliance with local regulations, and with appropriate air exchange for the work performed.

In the USA, OSHA 29 CFR Part 1910-1450 requires 4 to12 air changes per hour in laboratories.

WARNING! Biohazard: For biohazardous material use, always follow local regulations for hazard assessment, control, and handling. Neither the mass spectrometer nor any of its parts are intended to act as a biological containment safety cabinet.

Caution: Potential Mass Shift: Maintain a stable ambient temperature. If the temperature changes by more than 2°C, then the resolution and mass calibration will be affected.

Decommissioning and Disposal

Decontaminate the system before decommissioning following local regulations. Follow the AB SCIEX Red Tag process and complete an instrument Decontamination Form for instrument returns.

When removing the system from service, different materials must be separated and recycled according to national and local environmental regulations. Refer to Storage and Handling on page 129.

Do not dispose of system components or subassemblies, including computer parts, as unsorted municipal waste. Follow local municipal waste ordinances for proper disposal provisions to reduce the environmental impact of WEEE (waste, electrical, and electronic equipment). To make sure that you safely dispose of this equipment, contact an FSE for instructions.

European Union customers: Contact a local AB SCIEX Customer Service office for complimentary equipment pick-up and recycling.

Qualified Personnel

After installing the system, the AB SCIEX Field Service Employee (FSE) uses the *Customer Familiarization Checklist* to familiarize the customer with system operation, cleaning, and basic maintenance. Only qualified AB SCIEX personnel shall install and service the equipment. Only personnel qualified by AB SCIEX shall operate and maintain the equipment. Contact an FSE for more information.

Equipment Use and Modification

Use the system indoors in a laboratory that complies with the environmental conditions recommended in the system *Site Planning Guide*. If the system is used in an environment or in a manner not prescribed by AB SCIEX, the protection provided by the equipment can be impaired.

Unauthorized modification or operation of the system might cause personal injury and equipment damage, and might void the warranty. Erroneous data may be generated if the system is operating outside the recommended environmental conditions or with unauthorized modifications. Contact an AB SCIEX representative for more information on servicing the system.

This section lists the hazard symbols and conventions used in the laboratory environment, on the system, and in the documentation.

Occupational Health and Safety Symbols

This section describes some occupational health and safety symbols found in the documentation and laboratory environment.

Table 2-1 Electrical Hazard Symbols

Safety Symbol	Description
	Electrical Shock Hazard

Table 2-2 Chemical Hazard Symbols

Safety Symbol	Description
	Biohazard
	Explosion Hazard
	Toxic Chemical Hazard

Table 2-3 Mechanical Hazard Symbols

Safety Symbol	Description
	Hot Surface Hazard
	Laser Radiation Hazard
	Lifting Hazard
	Puncture Hazard

Table 2-3 Mechanical Hazard Symbols (Continued)

Safety Symbol	Description
	Radiation Hazard

Table 2-4 Pressurized Gas Hazard Warning Symbols

Safety Symbol	Description
	Pressurized Gas Hazard

Symbols, Indicators, and Labels

Packaging

Table 2-5 Labels on the Mass Spectrometer Shipping Materials

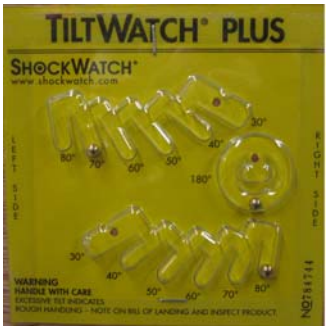
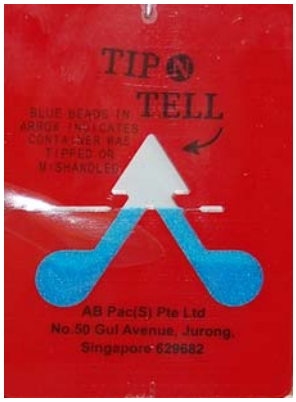
External Labels	Definition	Action
 	Tilt Indicator Indicates whether the container was tipped or mishandled.	Write on the Bill of Lading and check for damage. Any claims for tipping require a notation.

Table 2-5 Labels on the Mass Spectrometer Shipping Materials (Continued)

External Labels	Definition	Action
	Impact Indicator The indicator is activated if the container has suffered a shock greater than the level marked on the indicator.	Write on the Bill of Lading and check for damage. Any claims for shock damage require a notation.

Mass Spectrometer

Table 2-6 Labels on the Mass Spectrometer

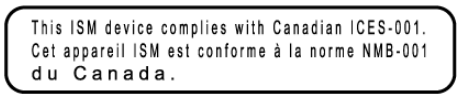
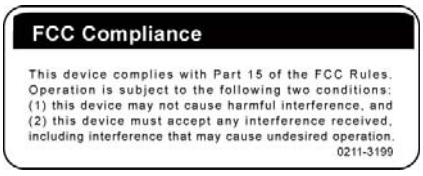
External Labels	Definition
	WARNING: NO USER SERVICEABLE PARTS INSIDE. REFER SERVICING TO QUALIFIED PERSONNEL.
	EN61326—1:2006 CLASS A, GROUP 1, ISM EQUIPMENT
	This ISM device complies with Canadian ICES-001. Cet appareil ISM est conforme à la norme NMB-001 du Canada.
	FCC Compliance. This device complies with Part 15 of the FCC Rules. Operation is subject to the following conditions: (1) this device may not cause harmful interference, and (2) this device must accept any interference received, including interference that may cause undesired operation.
	Do not dispose of equipment as unsorted municipal waste (WEEE).

Table 2-6 Labels on the Mass Spectrometer (Continued)

External Labels	Definition
FOR RESEARCH USE ONLY. NOT FOR USE IN DIAGNOSTIC PROCEDURES.	This system is for research use only. It is not intended for use in diagnostic procedures.
	Caution, refer to accompanying documents. Minimum of six persons required to safely lift this equipment.
	Consult operating instructions.
	Follow operating instructions (mandatory).
	Alternating Current
	High voltage. Electrical Shock Hazard
	On (Mains supply)
	Off (Mains supply)
	Protective Earth (ground)
V	Volts (voltage)
A	Amperes (current)

Documentation

The following symbols and conventions are used throughout the guide.

DANGER! Danger signifies an action which leads to severe injury or death.

WARNING! Warning signifies an operation that could cause personal injury if precautions are not followed.

Caution: Caution signifies an operation that could cause damage to the system or loss of data if precautions are not followed.

Tip! A tip provides useful information that helps apply the techniques and procedures in the text for a specific need, and provides shortcuts, but is *not essential* to the completion of a procedure.

Note: A note emphasizes significant information in a procedure or description.

AB SCIEX

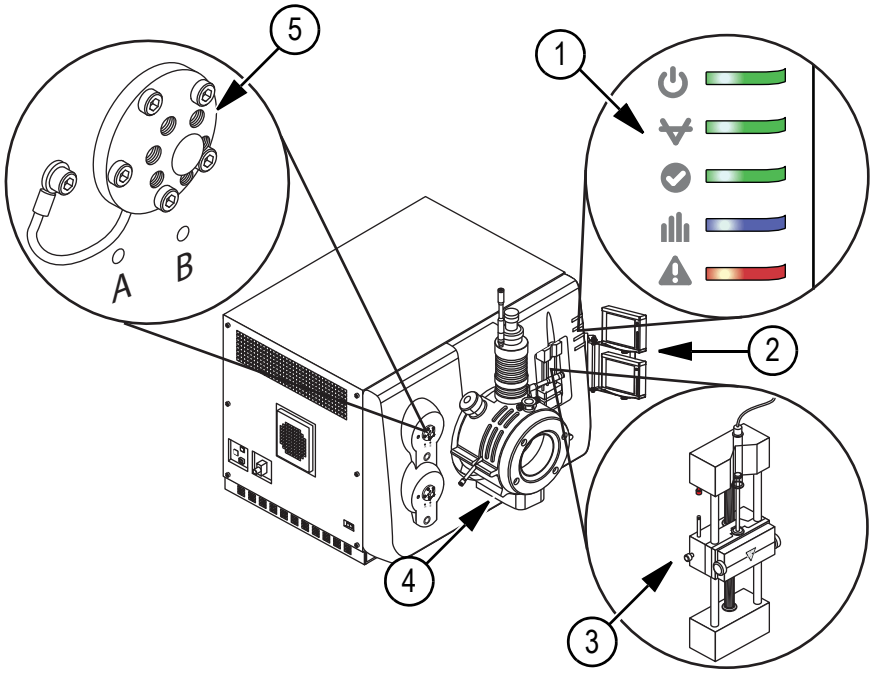
Principles of Operation 3

The 6500 series of instruments is intended for the qualitative and quantitative analysis of chemical species. The system includes a mass spectrometer, an optional bench, an IonDrive™ Turbo V ion source, a computer, and the Analyst® software.

System Overview

Figure 3-1 shows a system with a syringe pump, the ion source, a diverter valve, and the optional NanoSpray® ion source monitors.

Figure 3-1 Front View



Item	Description	For more information refer to...
1	Panel symbols	Table 3-1 on page 24.
2	Nanospray ion source monitors (optional)	*NanoSpray® Ion Source Operator Guide*, available from the ion source documentation CD, or from the AB SCIEX web site, at www.absciex.com
3	Syringe pump	Adjust the Integrated Syringe Pump Position on page 28.
4	Ion source	*IonDrive™ Turbo V Ion Source Operator Guide*, available from the ion source documentation CD, or from the AB SCIEX web site, at www.absciex.com

Item	Description	For more information refer to...
5	Diverter valve	Plumb the Diverter Valve on page 32. If the optional DuoSpray™ ion source is installed, then the diverter valve is replaced with the DuoSpray valve. The diverter valve is installed below the DuoSpray valve. For information about the DuoSpray ion source, refer to the *DuoSpray™ Ion Source Operator Guide*, available from the ion source documentation CD, or from the AB SCIEX web site, at www.absciex.com

Panel Symbols

Table 3-1 shows the mass spectrometer status LEDs.

Table 3-1 Panel Symbols

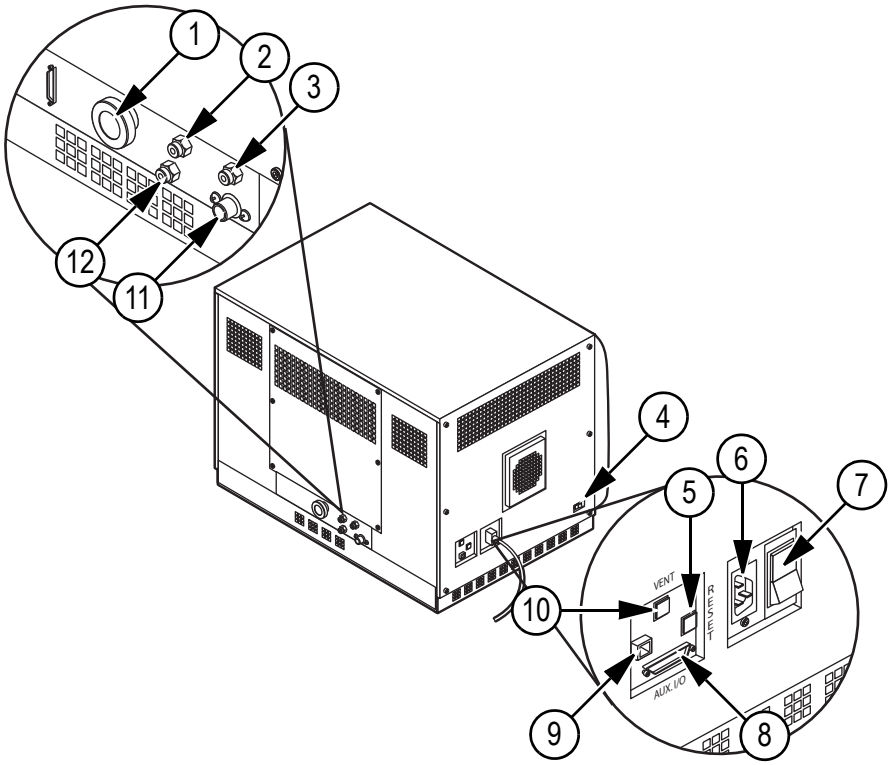
LED	Color	Name	Description
	Green	Power	Lit when the system is powered up.
	Green	Vacuum	Lit when the correct vacuum has been achieved. Flashing if the vacuum is not at the correct vacuum (during pumpdown and venting.)
	Green	Ready	Lit when the system is in the Ready state. The system must be in the Ready state to operate.
	Blue	Scanning	Flashing when the system is acquiring data.
	Red	Fault	Lit when the system encounters a system fault.

After the system is turned on, all five LEDs illuminate. The power LED remains lit. The other four LEDs flash for two seconds and then turn off. The vacuum LED starts flashing. After the correct vacuum has been achieved this LED remains lit.

Connections

Figure 3-2 shows the location of the mass spectrometer connections, including the locations of the **Reset** and **Vent** buttons and the mass spectrometer switch.

Figure 3-2 Change and Side Views



Item	Description	For more information...
1	Roughing pump vacuum connection	Contact an FSE.
2	Nitrogen gas supply (Curtain Gas™ supply, CAD gas)	Contact an FSE.
3	Source exhaust supply	Contact an FSE.
4	Source communication connection	Contact an FSE.
5	**Reset** button	Refer to Reset the System on page 27.
6	Mains supply connection	Refer to Start Up the System on page 27 or Shut Down the System on page 28.
7	Mass spectrometer switch (Up = On; Down = Off)	Refer to Start Up the System on page 27 or Shut Down the System on page 28.
8	Aux I/O connection	Refer to the *Peripheral Devices Setup Guide*.
9	Ethernet connection (connects the mass spectrometer and the computer)	Contact an FSE.
10	**Vent** button	Refer to Start Up the System on page 27 or Shut Down the System on page 28.
11	Source exhaust waste (to waste bottle)	Contact an FSE.
12	Air supply (Gas1/Gas2)	Contact an FSE.

Theory of Operation

Mass spectrometry measures the mass-to-charge ratio of ions to identify unknown compounds, to quantify known compounds, and to provide information about the structural and chemical properties of molecules.

The 6500 series of instruments has a series of quadrupole filters that transmit ions according to their mass-to-charge (m/z) ratio. The first quadrupole in this series is the QJet® ion guide, which is located between the orifice plate and the Q0 region. The QJet ion guide does not filter ions, but focuses them before they enter the Q0 region. By prefocusing the larger ion flux created by the wider orifice, the QJet ion guide increases system sensitivity and improves the signal-to-noise ratio. In the Q0 region, the ions are again focused before passing into the Q1 quadrupole.

The Q1 quadrupole is a filtering quadrupole that sorts the ions before they enter the Q2 collision cell. The Q2 collision cell is where the internal energy of an ion is increased through collisions with gas molecules to the point that molecular bonds break creating product ions. This technique allows users to design experiments that measure the m/z of product ions to determine the composition of the parent ions.

After passing through the Q2 collision cell, the ions enter the Q3 quadrupole for additional filtering, and then enter the detector. In the detector, the ions create a current that is converted into a voltage pulse. The voltage pulses leaving the detector are directly proportional to the quantity of ions entering the detector. The system monitors these voltage pulses and converts the information into a signal. The signal represents the ion intensity for a particular m/z value and the system displays this information as a mass spectrum.

Data Handling

The Analyst software requires a computer running the Windows operating system. The computer with the associated system software works with the system controller and associated firmware to control the system and data acquisition. During system operation, the acquired data is sent to the Analyst software where it can be displayed as either full mass spectra, intensity of single or multiple ions versus time, or total ion current versus time.

Start Up the System

WARNING! Lifting Hazard: Risk of personal injury or system damage. If the system must be moved, contact an FSE.

Note: Before operating the system, read the safety information in the Operational Precautions and Limitations on page 9.

Before the system is turned on, make sure the site requirements specified in the *Site Planning Guide* are met. This guide includes information on the site layout, electrical, gas supply, ventilation and waste collection, and environmental requirements.

1. Make sure that there is clear access to the AC mains supply cable. The AC mains supply cable must be accessible in order to disconnect the mass spectrometer from the AC mains supply.
2. Make sure that the 4 L source exhaust drain bottle is connected to the Exhaust Waste connection on the rear of the mass spectrometer and to the laboratory ventilation system.
3. Make sure that the AC mains supply cable is plugged in to the mass spectrometer.
4. Make sure that the mass spectrometer and roughing pump AC mains supply cables are plugged into the AC mains supply.
5. Make sure that the Ethernet cable is connected to both the mass spectrometer and the computer.
6. Turn on the mass spectrometer switch.

   Note: If the switch is already on, turn it off and then on.

   The mass spectrometer starts, and then the roughing pump starts up after 30 seconds.
7. Turn on the computer, if it was turned off.
8. Start the Analyst® software.

Reset the System

- Press and hold the **Reset** button for 5 seconds.

  An audible click is heard when the relay activates. After approximately three minutes, the mass spectrometer should reach operating pressure.

Shut Down the System

Tip! If the mass spectrometer will not be used for a length of time, we recommend that it be left in standby with the ion source in place. If the mass spectrometer must be shut down, follow these instructions. Do not turn off the roughing pump until after the turbo pumps have spun down.

1. Complete or stop any ongoing scans. For more information, refer to Stop Sample Acquisition on page 71.
2. Turn off the sample flow to the system.

   Caution: Potential System Damage: Turn off the sample flow before the system is shut down.
3. In the Analyst software, deactivate the hardware profile, if it is active.
4. Close the software.
5. Press and hold the **Vent** button for three seconds.

   The turbo pump will spin down gradually. The roughing pump is controlled by the mass spectrometer and will continue to run for approximately 15 minutes.
6. Wait 15 minutes, then turn off the mass spectrometer switch.
7. Unplug the mass spectrometer and roughing pump AC mains supply cables from the AC mains supply.
8. Unplug the AC mains supply cable from the bulkhead on the left side of the mass spectrometer.

Adjust the Integrated Syringe Pump Position

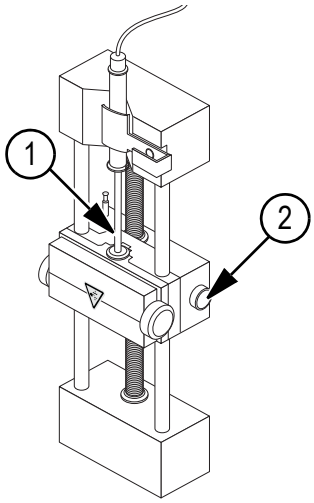
WARNING! Personal Injury Hazard: Make sure that the syringe is seated properly in the syringe pump and the automatic syringe pump stop is adjusted properly to avoid damaging or breaking the glass syringe.

WARNING! Puncture Hazard: Take care when inserting the syringe. The tip of the syringe is extremely sharp.

1. Press the **Release** button on the right side of the syringe pump to lower the base and then insert the syringe.

   Make sure that the end of the syringe is flush against the base and that the shaft of the syringe rests in the cutout.

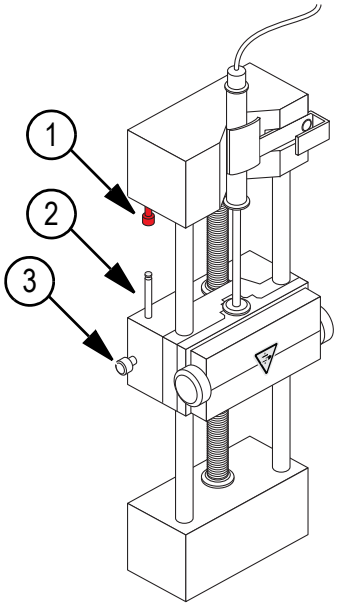
Figure 4-1 Lowering the Base



Item	Description
1	Syringe plunger.
2	Release button. Press to raise or lower the base.

2. Adjust the post so that it triggers the automatic syringe stop before the syringe plunger hits the bottom of the glass syringe.

Figure 4-2 Safety Stop

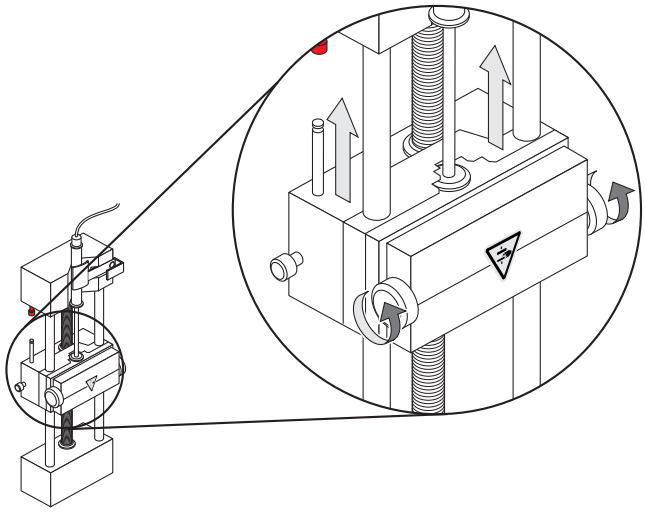


Item	Description
1	Automatic syringe stop. After the post hits the automatic syringe stop, the syringe pump stops.

Item	Description
2	Post. Adjust the height to prevent the syringe plunger from hitting the syringe during sample infusion.
3	Post lock screw. Tighten the screw after the height of the post is adjusted.

3. Turn the side screws to secure the syringe.

Figure 4-3 Turning the Side Screws

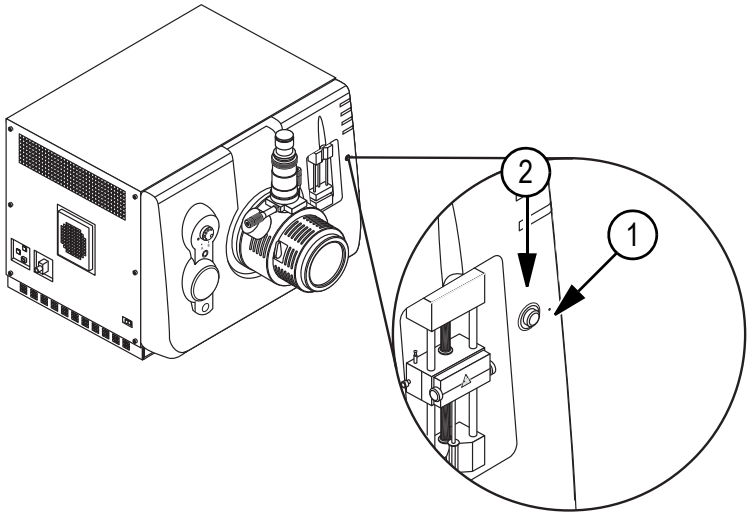


4. On the mass spectrometer, press the button on the right side of the syringe pump to start the flow.

   The green light next to the button illuminates when the syringe pump is in use.

Tip! The syringe pump can also be started using the Analyst software in Manual Tuning mode.

Figure 4-4 Syringe Pump Button and LED



Item	Description
1	Syringe pump status LED
2	Syringe pump on/off button

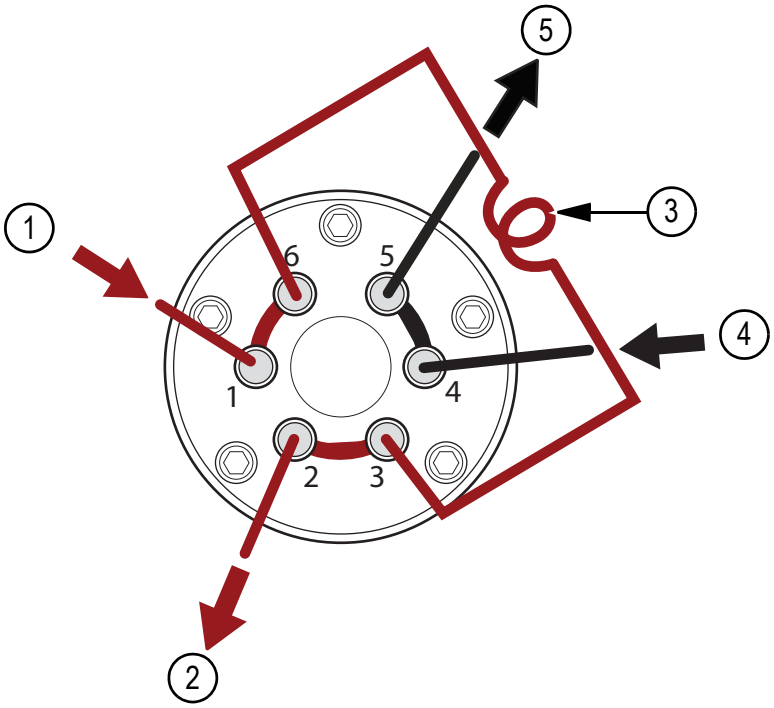
Plumb the Diverter Valve

Plumb the diverter valve for both injector and diverter modes.

Plumb the Diverter Valve in Injector Mode

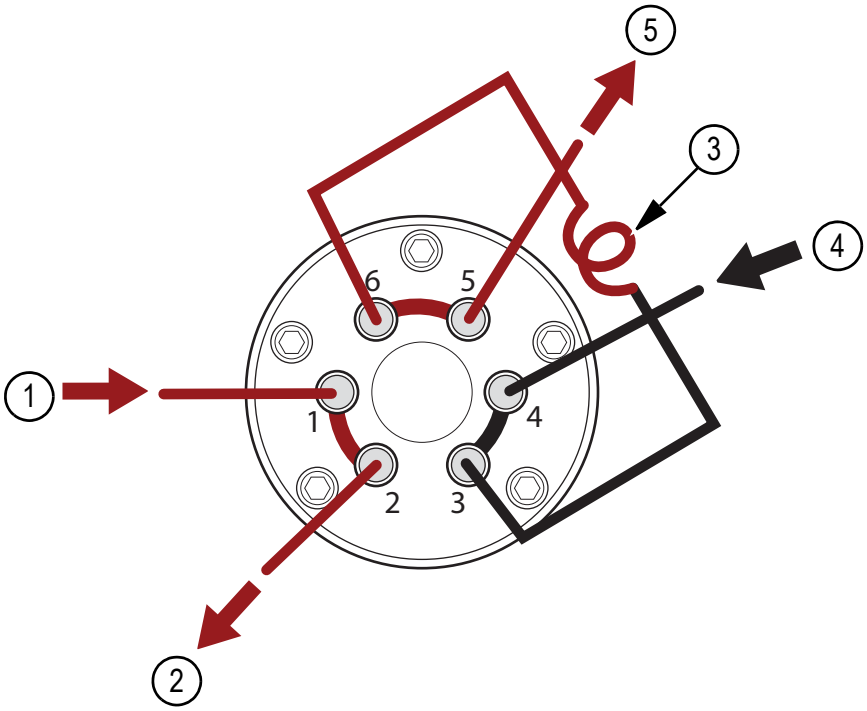
The diverter valve is a two position, 6 port valve. If you put the valve in Position A (Figure 4-5), the sample flows through the external loop. When you switch the valve to Position B (Figure 4-6), the sample is injected.

Figure 4-5 Diverter Valve—Injector Mode Position A



Item	Description
1	Sample in
2	Waste out
3	Sample loop
4	Mobile phase in
5	To column

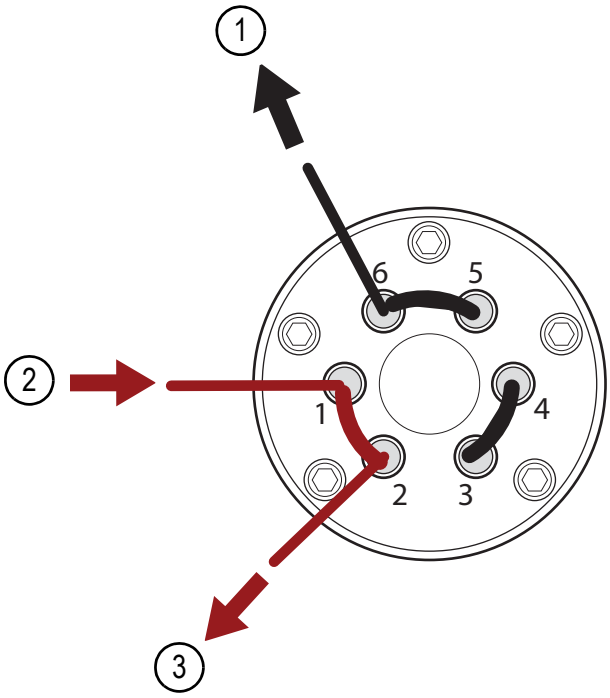
Figure 4-6 Diverter Valve—Injector Mode Position B



Item	Description
1	Sample in
2	Waste out
3	Sample loop
4	Mobile phase in
5	To column

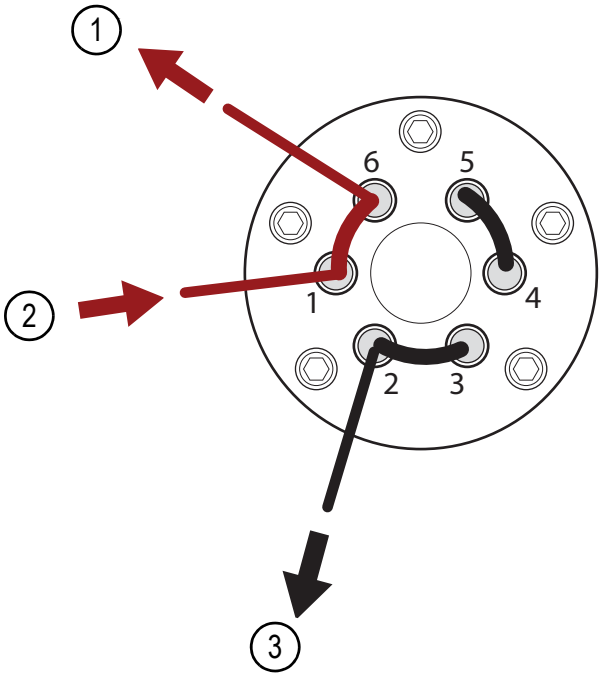
Plumb the Diverter Valve in Diverter Mode

Figure 4-7 Diverter Valve—Diverter Mode Position A



Item	Description
1	To mass spectrometer
2	From column
3	Waste out

Figure 4-8 Diverter Valve—Diverter Mode Position B



Item	Description
1	To mass spectrometer
2	From column
3	Waste out

Table 5-1 Instrument Setup

Step	To do this...	Find the information in...	What does it do?
1	Create a hardware profile.	Create a Hardware Profile on page 39	Each hardware profile must include a mass spectrometer. Only devices included in the active hardware profile can be used when creating acquisition methods.
2	Create projects to store data.	Projects and Subprojects on page 46	Before starting an experiment, decide where to store the files related to the experiment. Using projects and subprojects improves data management and makes comparison of results easier.
3	Optimize the mass spectrometer.	Optimize the Instrument on page 51	This is the process of optimizing the resolution and mass spectrometer parameters, and calibrating the mass spectrometer to obtain the best sensitivity and performance from the system.

Table 5-2 Sample Acquisition Workflow

Step	To do this...	Find the information in...	What does it do?
1	Create projects to store data.	Projects and Subprojects on page 46	Before starting an experiment, decide where to store the files related to the experiment. Using projects and subprojects improves data management and makes comparison of results easier.
2	Create an acquisition method.	Create Acquisition Methods on page 55	To analyze samples, create an acquisition method for the mass spectrometer and any LC devices. An acquisition method indicates which peripheral devices to use, when to use them to acquire data, and the associated parameters.
3	Create and submit a batch.	Add Sets and Samples to a Batch on page 66 and Submit a Sample or Set of Samples on page 68	After creating an acquisition method, run samples by creating an acquisition batch and submitting the batch to the Acquisition Queue.

Table 5-2 Sample Acquisition Workflow (Continued)

Step	To do this...	Find the information in...	What does it do?
5	Acquire data.	Acquire Data on page 68	Running samples involves managing the acquisition queue and monitoring instrument and device status. To submit samples and acquire data, use the Queue Manager. The Queue Manager displays queue, batch, and sample status, and facilitates management of samples and batches in the queue.
6	Analyze data in Explore mode. **—OR—** Analyze quantitative data	Operating Instructions — Analyze and Process Data on page 79 Operating Instructions — Analyze and Process Quantitative Data on page 97	In Explore mode, many tools are available for viewing and processing the acquired data. Graphs can be customized with peak labels and captions, contour plots can be displayed, and spectra can be saved in the library. Use the various quantitative method creation tools in Quantitate mode to analyze the acquired data and build a quantitative method to generate a Results Table. Use the Results Table to manually review all of the peaks for each analyte and internal standard within a batch and to view calibration curves, sample statistics, and metric plots.

Hardware Profiles

A hardware profile tells the software which mass spectrometer and devices to use, and how the instrument and the devices are configured and connected to the computer.

Each hardware profile must include a mass spectrometer. Before creating an acquisition method, make sure that all devices used in the method are included in the hardware profile. In the configuration options for the mass spectrometer, make sure that the syringe pump is enabled if it will be used during acquisition.

The devices configured in the active hardware profile and selected in the Add/Remove Device Method dialog appear as icons in the Acquisition Method Browser pane. Only devices included in the active hardware profile can be used to create acquisition methods.

For information about setting up the physical connections to the devices, refer to the *Peripheral Devices Setup Guide*. For a list of the supported devices, refer to the *Software Installation Guide* for the Analyst® software.

Create a Hardware Profile

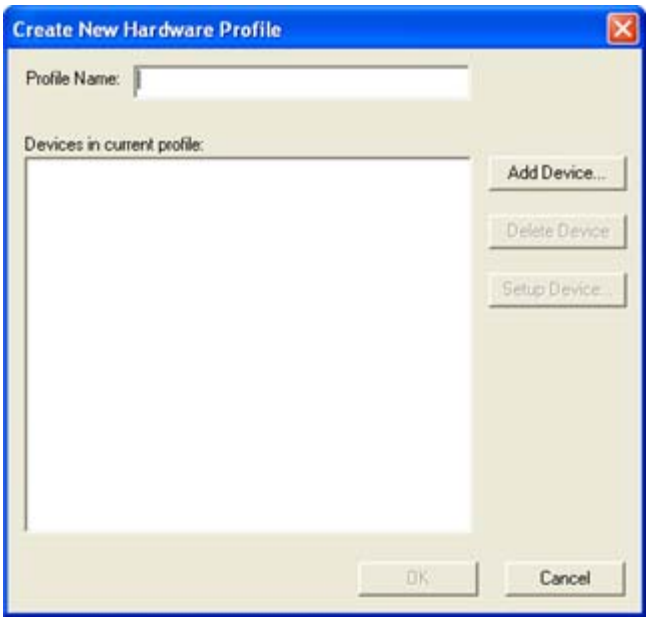
The user can create multiple hardware profiles, but only one profile can be active at any time. In the hardware profile, users can specify the mass range in which the 6500 series of instruments should operate.

1. In the navigation bar, under **Configure**, double-click **Hardware Configuration**.

Figure 6-1 Hardware Configuration Editor Dialog

2. In the **Hardware Configuration Editor** dialog, click **New Profile**.

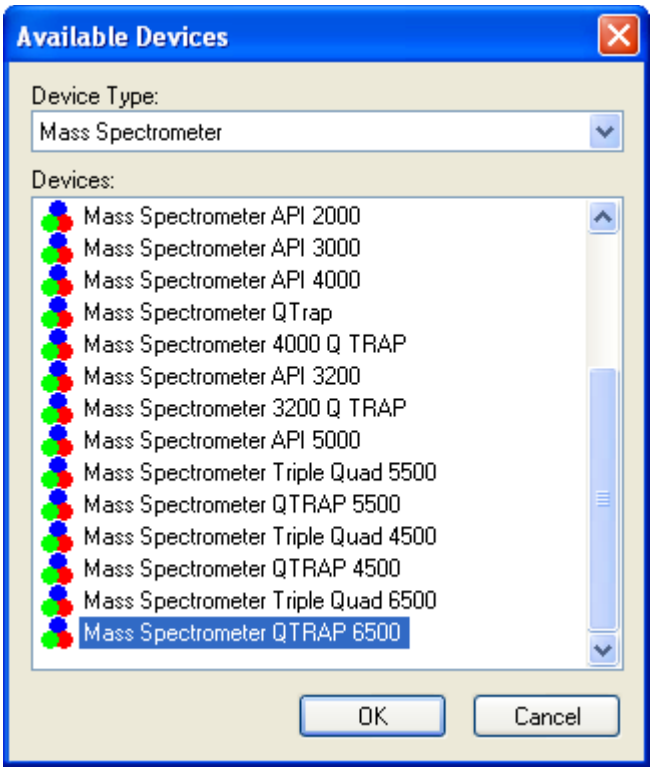
Figure 6-2 Create New Hardware Profile Dialog



3. In the **Profile Name** field, type a name.
4. Click **Add Device**.

   In the **Available Devices** dialog, in the **Device Type** field, **Mass Spectrometer** is the preset value.
5. In the **Devices** list, select the mass spectrometer.

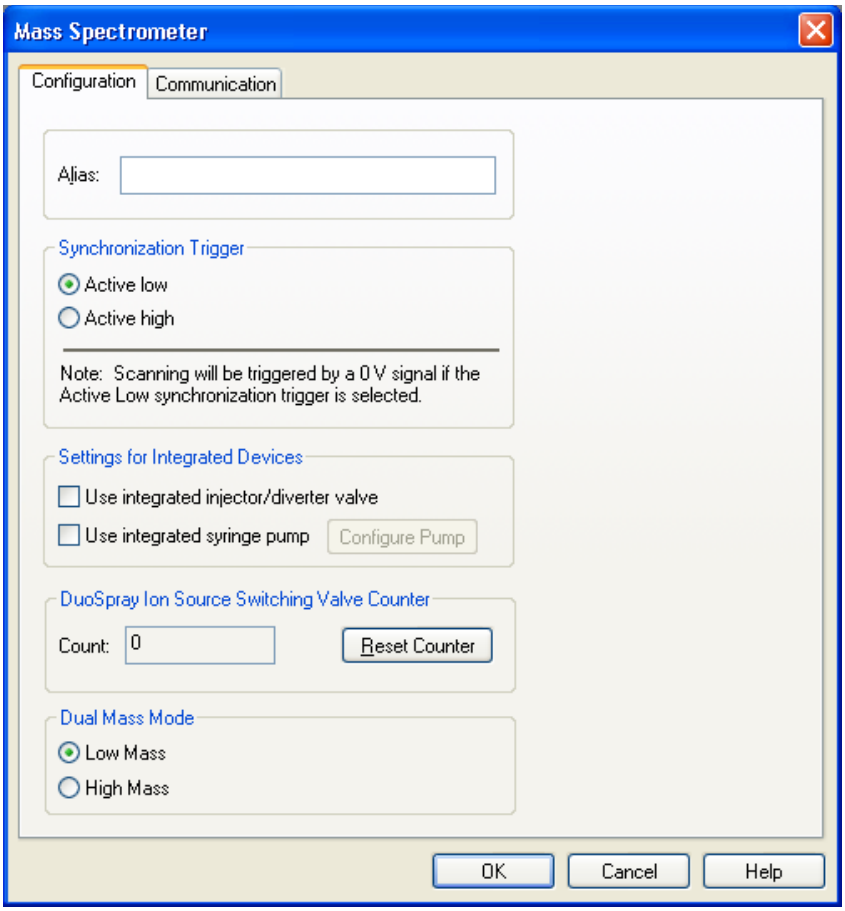
Figure 6-3 Available Devices Dialog



6. Click **OK**.
7. In the **Devices in current profile** list, select the mass spectrometer.
8. Click **Setup Device**.

   The **Mass Spectrometer** dialog opens.

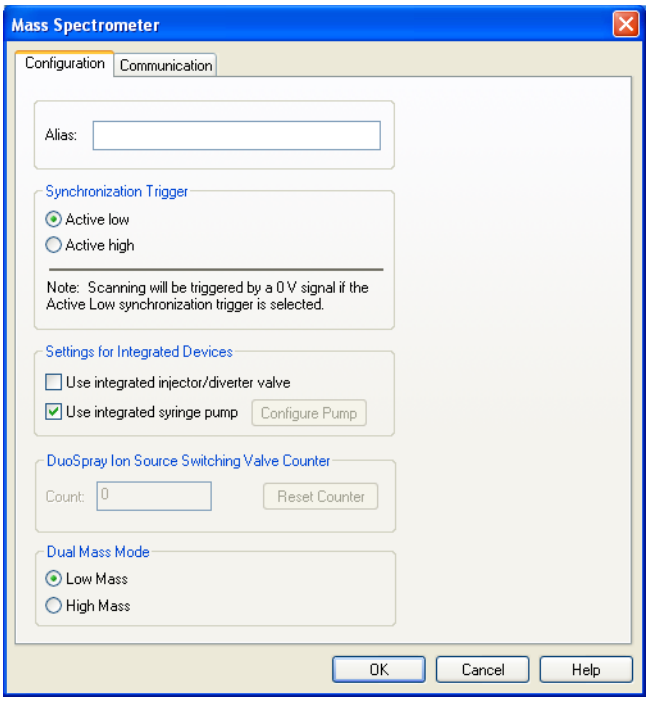
Figure 6-4 Mass Spectrometer Dialog: Configuration Tab



9. On the **Configuration** tab, in the **Dual Mass Mode** section, select one of the following two options:
   - **Low Mass**: To operate in limited mass range, high sensitivity operating mode, select this option. The mass range is 5 to 1000 Da for LIT (linear ion trap) scans and 50 to 1250 Da for quadrupole scans.
   - **High Mass**: To operate in extended mass range operating mode, select this option.The mass range is 5 to 2000 Da for LIT scans and 50 to 2000 Da for quadrupole scans.
10. (Optional) To configure the mass spectrometer for the integrated syringe pump, on the **Configuration** tab, select **Use integrated syringe pump**.

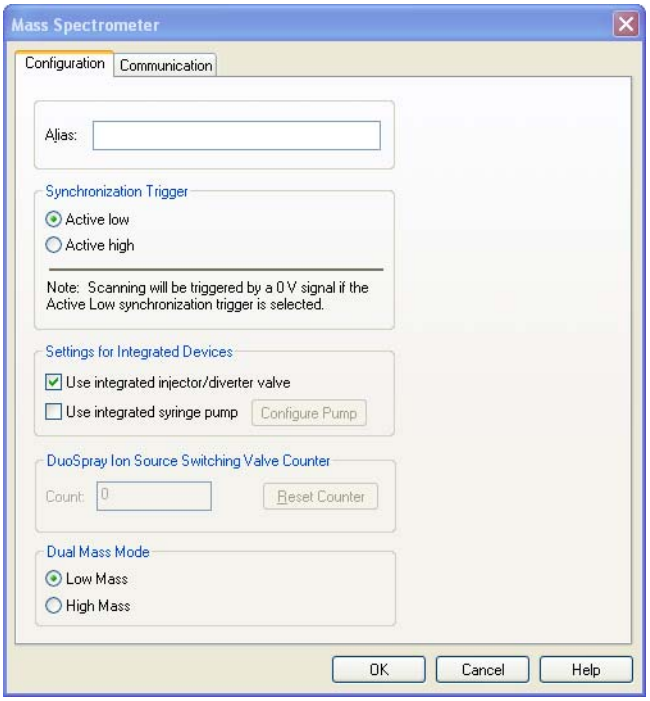
WARNING! Personal Injury Hazard: Make sure that the syringe is seated properly in the syringe pump and the automatic syringe pump stop is adjusted properly to avoid damaging or breaking the glass syringe.

Figure 6-5 Configuration Tab with Syringe Pump Configured



11. (Optional) To configure the mass spectrometer for the diverter valve, on the **Configuration** tab, select **Use integrated injector/diverter valve**.

Figure 6-6 Configuration Tab with Diverter Valve Configured



12. Select additional features on the **Configuration** and **Communication** tabs as required.

13. Click **OK** to return to the **Create New Hardware Profile** dialog.
14. Add and configure each device that is used with the instrument. Refer to step 4 on page 44.
15. In the **Create New Hardware Profile** dialog, click **OK**.
16. In the **Hardware Configuration Editor**, click the hardware profile.
17. Click **Activate Profile**.

    The check mark turns green. If a red x is shown, then there is an issue with the hardware profile activation. For more information, refer to Troubleshoot Hardware Profile Activation.

Tip! A hardware profile does not have to be deactivated before another is activated. Click a hardware profile and then click **Activate Profile**. The other profile is deactivated automatically.

18. Click **Close**.

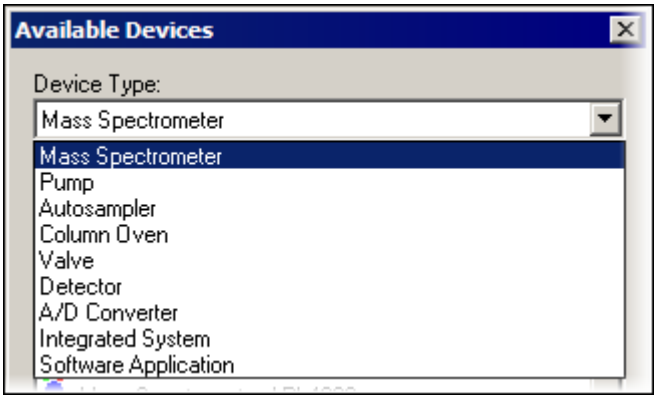
Add Devices to a Hardware Profile

Devices must be configured to enable the software to communicate with them.

When the software is installed, the driver required for each device is also installed. After the devices are physically connected to the computer, configure the device.

1. Open the **Hardware Configuration Editor**.
2. In the **Hardware Profiles** list, deactivate the hardware profile.
3. Click **Edit Profile**.
4. Click **Add Device**.
5. In the **Available Devices** dialog, in the **Device Type** list, select the device.
6. Click **OK**.

Figure 6-7 Available Devices Dialog



7. In the **Devices in current profile** list, select the device.
8. Click **Setup Device**.

   A dialog containing configuration values for the device opens.

9. (Optional) On the **Communication** tab, in the **Alias** field, type a name or other identifier.

Note: For devices using serial communication, make sure that the serial port selected matches the serial port to which the device is physically connected. If a serial expansion cable is used, then the number selected in the profile is the number on the cable plus two.

Note: The **Alias** field may also be referred to as the Name box and may be found on another tab under **Alias**.

- If the device uses **Serial Port** as a communication interface, in the **COM Port Number** list, select the COM port to which the device is connected.
- If the device uses **Ethernet** as a communication interface, type the **IP Address** assigned to the device by the administrator or use the corresponding **Host Name** for the address.
- If the device uses **GPIB Board** as a communication interface, do not change the settings for the GPIB board.

The rest of the preset values for the device are probably appropriate. Do not change them. For information about the **Configuration** and **Communication** tabs, refer to the Help.

10. To restore the device preset values, on the **Communication** tab, click **Set Defaults**.
11. To save the configuration, click **OK**.
12. Repeat step 4 to step 11 for each device.
13. In the **Create New Hardware Profile** dialog, click **OK**.
14. To activate the hardware profile, in the **Hardware Configuration Editor**, click the hardware profile.
15. Click **Activate Profile**.

    The check mark turns green. If a red x is shown, then there is an issue with the hardware profile activation. For more information, refer to Troubleshoot Hardware Profile Activation.

Tip! A hardware profile does not have to be deactivated before activating another hardware profile. Click a hardware profile and then click **Activate Profile**. The other profile is deactivated automatically.

16. Click **Close**.

Troubleshoot Hardware Profile Activation

If a hardware profile fails to become active, a dialog appears indicating which device in the profile failed. A failed profile may be due to communications errors.

1. Read the error message generated. Depending on the message, there may be an issue with a device or how the communication is set up.
2. Verify that the device has power and is turned on.

3. Verify that the COM port assigned to the device is correct.

Tip! On computers with two built-in serial ports, the first port on the serial port expansion card is usually COM3, even though the cable indicates P1.

4. Verify that the communication settings with the device (for example, dip switch settings) are set correctly and match the settings on the **Communication** tab.
5. Turn off the device.
6. Wait 10 seconds
7. Turn on the device.

   Wait until all device power-up activities are complete before trying to activate the hardware profile again. Some devices may require 30 seconds or more to complete the power-up activities.
8. Activate the hardware profile.
9. If the issue persists, delete the failing profile and then create a new one.
10. If the issue persists, contact technical support.

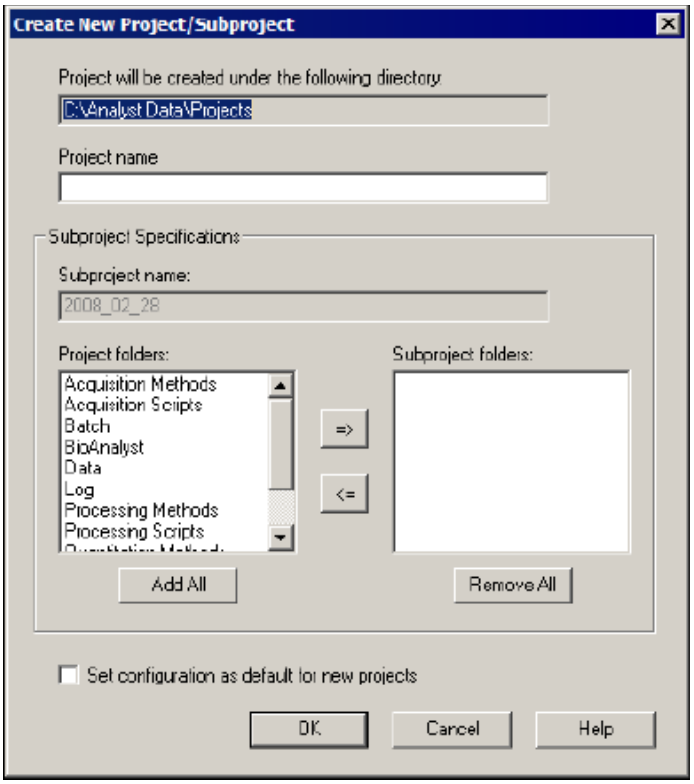
Projects and Subprojects

Create Projects and Subprojects

To use a subproject structure within a project, create the subproject structure when the project is created.

1. Click **Tools > Project > Create Project**.
2. In the **Project name** field, type a project name.
3. (Optional) To use subprojects, select the required folders and then use the arrow buttons to move them to the **Subproject folders** list.

Figure 6-8 Create New Project/Subproject Dialog



4. (If subprojects are used) In the **Subproject name** field, type a name for the first subproject or use the existing date.
5. (Optional) To use this project and subproject folder organization for all new projects, select the **Set configuration as default for new projects** check box.

   All new projects are created with this folder configuration.
6. Click **OK**.

Create Subprojects

Subprojects can only be created in a project that has an existing subproject structure.

1. On the Project toolbar, in the **Project** list, select the project.
2. Click **Tools > Project > Create Subproject**.
3. In the **Subproject name box**, type a name for the subproject or use the existing date.
4. Click **OK**.

Copy Subprojects

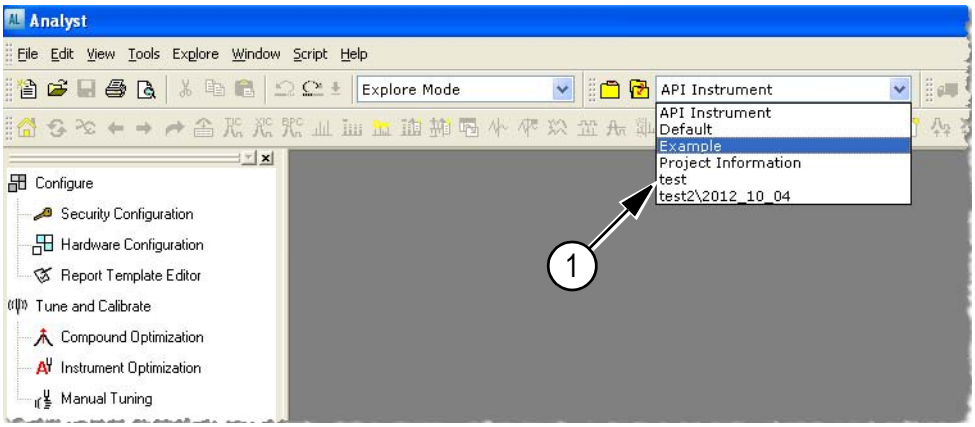
A subproject can be copied from another project that has existing subprojects. If the copied subprojects contain folders that also exist in the project folder, then the software uses the project level folders.

1. Click **Tools > Project > Copy Subproject**.
2. In the **Copy Subproject** dialog, click **Browse** to navigate to the subproject source.
3. Click **OK**.
4. In the **Source Subproject** list, select the subproject.
5. Click **Browse** to navigate to the subproject destination.
6. In the **Target Subproject** field, type the name.
7. Click **OK**.
8. Do one of the following:
   - To copy all folders and files from the **Subproject Source** into the **Subproject Destination**, select the **Copy Contents** check box.
   - To copy only the folders in the same structure into the **Subproject Destination**, make sure that the **Copy Contents** check box is cleared.
9. Click **Copy**.

Switch Between Projects and Subprojects

- On the software toolbar, from the project list, click the required project or subproject.

Figure 6-9 Project List



Item	Description
1	Project list showing a folder, Tutorial, and the Tutorial folders subfolders.

Table 6-1 Icons on the Toolbar

Icon	Name	Function
	New Subproject	Creates a subproject. Subprojects can only be created later in the process if the project was originally created with subprojects.

Table 6-1 Icons on the Toolbar (Continued)

Icon	Name	Function
	Copy Subproject	Copies a Subproject folder. Subprojects can be copied only from another project that has existing subprojects. If the same folders exist at both the project and subproject levels, the software uses the project level folders.

Installed Project Folders

Three project folders are installed with the software: API Instrument, Default, and Example.

API Instrument Folder

The **API Instrument** folder is unique and very important to the correct functioning of the mass spectrometer. The **API Instrument** folder contains the information required for tuning and calibrating the mass spectrometer. This information includes parameter settings files, reference files, instrument data files that contain calibration and resolution information, and the acquisition methods used during automatic tuning. The **API Instrument** folder also contains data files for manual tuning runs that were performed using the **Start** button rather than the **Acquire** button. These data files are saved automatically in the **API Instrument** folder in the **Tuning Cache** folder and named with the date and time they were created. The **Tuning Cache** folder is automatically cleared periodically.

Default Folder

The **Default** folder contains folders that are present in new projects and serves as a template for new projects.

Example Folder

The **Example** folder contains sample methods and data files. Users can practice working with the Explore or Quantitate modes using the example data files. The example files are sorted into subfolders by mass spectrometer type and application area.

Back Up the API Instrument Folder

Back up the **API Instrument** folder regularly and after routine maintenance has been performed.

1. Copy the **API Instrument** folder, paste it to a different location, preferably to another computer, and then rename the folder. Use the date and a mass spectrometer reference if there is more than one mass spectrometer when the folder is named. For example, API Instrument__4000QTRAP3_010107
2. To recover the folder, rename the current **API Instrument** folder, copy the backup folder into the **Projects** folder, and then change the name of the backup folder to **API Instrument**.

Run the Verify instrument performance option weekly or after the mass spectrometer is cleaned to confirm that the system is working properly. In general, for triple quadrupole systems, calibration and resolution is satisfactory for three to six months unless the system loses vacuum. For linear ion trap (LIT) systems, the resolution should also be satisfactory for three to six months but the system should be calibrated approximately monthly. If the system loses vacuum, then check the calibration and resolution before using the system. For more information about tuning and calibration, refer to the *Advanced User Guide* and the *Manual Tuning Tutorial*.

Tip! Perform maintenance tasks regularly to make sure that the mass spectrometer is performing optimally. Refer to Table 14-1 on page 131.

Required Materials
• Tuning solutions that are supplied in the Standards Chemical Kit shipped with the system. If needed, a new kit can be ordered from AB SCIEX.
• 5 mL, 1 mL, and 250 µL serial gas-tight syringes.
• red PEEK sample tubing.

Prerequisites
• A printer is configured.
• The spray is stable and the correct tuning solution is being used.

Optimize the Instrument

The following procedure describes how to verify the performance of the instrument. For more information about using the other instrument performance options, refer to the Help.

1. In the navigation bar, under **Tune and Calibrate**, double-click **Manual Tuning**.
2. Run a calibration method, and confirm that the TIC is stable and that the peaks of interest are present in the spectrum.
3. In the navigation bar, under **Tune and Calibrate**, double-click **Instrument Optimization**.

   The **Instrument Optimization** dialog opens.

   The instrument name and the current operating mode configured in the active hardware profile is shown at the bottom of the dialog.
4. Click **Verify instrument performance**.
5. Click **Next**.
6. Click **Approved Tuning**.
7. Click **Next.**

8. Select a **Tuning Solution**.

   Depending on the solution selected, different modes are available.

   i. Click a polarity.
   ii. If available, click **Q1** and **Q3** in the **Quad** section. If available, click the required scan speeds.
   iii. If available, click the scan speeds in the **LIT** section.
   iv. If available, click **Excitation** in the MS/MS/MS section.

9. Click **Next**.
10. If the **Select a mode** page opens, select **Automatic**.
11. Click **Next**.
12. Click **GO**.

    The **Verifying or Adjusting Performance** screen opens. After the process has completed, the **Results Summary** opens. For more information, refer to the Help.

13. If applicable (depending on the options selected), change solutions when prompted.

Verify or Adjust Performance

The top left corner shows the part of the instrument that is being tuned.

Current Spectrum: This graph shows the spectrum of the current scan, the optimal scan selected by the software, or the scan at the current parameter value when the software results are viewed in interactive mode.

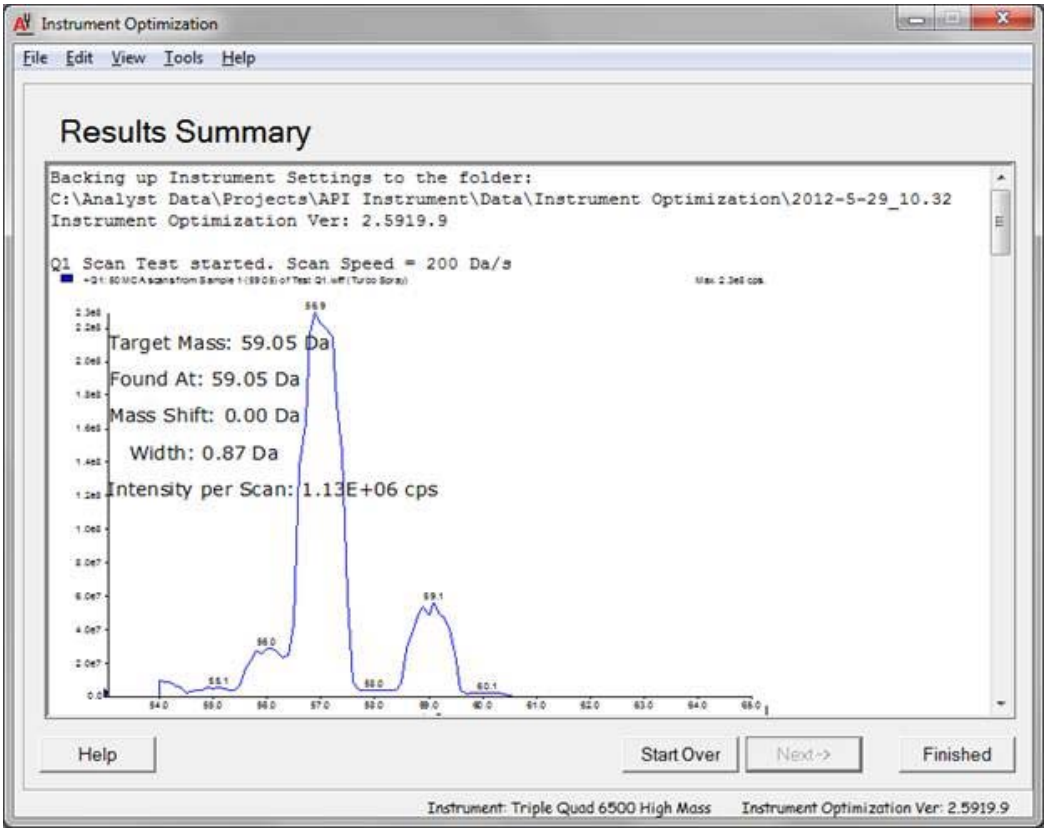
The **Instrument Optimization Decision Plots**, in the top right graph, dynamically show the intensity versus voltage curves of the parameters that are currently being optimized.

Results Summary

The **Results Summary** is a record of any instrument settings changes that were made by the Instrument Optimization software. Refer to the **Results Summary** shown in Figure 7-1 on page 53. This includes the location of data files and instrument settings backups, as well as step-by-step changes and results during optimization.The **Results Summary** also shows a verification report. This report contains a snapshot of the mass spectrum for each relevant mass for the scan modes being verified. The spectrum is labelled with the target mass, where the mass was found, mass shift, peak width, and peak intensity. The spectrum can be used as a visual record of peak shape or scan mode performance. A summary table of results follows the spectra.

The **Results Summary** is saved as a document in the folder indicated at the top of the report. Users can print the **Results Summary** or open a previously saved **Results Summary**.

Figure 7-1 Results Summary



An acquisition method consists of experiments and periods. Use the **Acquisition Method** editor to create a sequence of periods and experiments for the instrument and devices.

Create Acquisition Methods

Only devices configured in the active hardware profile appear in the **Acquisition method** pane. Any devices added to the hardware profile must also be added to existing acquisition methods. For more information about devices, refer to the *Peripheral Devices Setup Guide.*

1. In the navigation bar, under **Acquire**, double-click **Build Acquisition Method**.
2. In the **Acquisition Method Properties** tab, select a **Synchronization Mode**.
3. (Optional) Select the **Auto-Equilibration** check box and then type the desired equilibration time, in minutes.
4. In the **Acquisition method** pane, click the **Mass Spec** icon.
5. On the **MS** tab, select a scan type.
6. Type values in the fields as required. Refer to Parameters on page 58.
7. On the **Advanced MS** tab, type values in the fields as required. Refer to Parameters on page 58.
8. Click a device icon and then select the parameters for the device. To configure the syringe pump, refer to Configure the Syringe Pump on page 55.
9. Add any additional periods and experiments. Refer to Add an Experiment on page 55 and Add a Period on page 56
10. Click **File** > **Save**.

Configure the Syringe Pump

1. In the **Acquisition method** pane, click the **Syringe Pump** icon.

   The **Syringe Pump Method Properties** tab opens in the **Acquisition Method** editor pane.
2. In the **Syringe Diameter (mm)** field, type the syringe diameter.
3. In the **Flow Rate** field, type the flow rate.
4. In the **Unit** list, select the units of flow.

Add an Experiment

1. Right-click the period and then click **Add experiment**.

   An experiment is added below the last experiment in the period.
2. In the **Acquisition Method Editor** pane, select the appropriate device or instrument parameters.

Add a Period

- In the **Acquisition method** pane, right-click the **Mass Spec** icon, and then click **Add period**.

  A period is added below the last period created.

Copy an Experiment into a Period

Prerequisite Procedures
• Open a multi-period method

- In the **Acquisition method** pane, press CTRL, and then drag the experiment to the period.

  The experiment is copied below the last experiment in the period.

Copy an Experiment within a Period

Use this procedure to add the same or similar experiments to a period if most or all of the parameters are the same.

- Right-click the experiment and then click **Copy this experiment**.

Scan Techniques

MS: In MS scans, also referred to as single MS scans, ions are separated according to their mass-to-charge (*m/z*) ratio. A single MS scan may be used to determine the molecular weight of a compound. Single MS scans can also be referred to as survey scans. MS scans do not provide any information as to the chemical make-up of the ions other than the *m/z* ratio. Perform MS/MS or MS/MS/MS scan types to obtain more information about the ions.

MS/MS: MS/MS scans are used to help identify or confirm a molecular species. In MS/MS scans, a precursor ion can be fragmented in one of two locations.

- For triple quadrupole systems, fragmentation occurs in the collision cell.
- For LIT systems, fragmentation can occur in the collision cell or the linear ion trap.

If enough energy is used, the precursor ion fragments to produce characteristic product ions.

MS/MS/MS: The LIT instrument MS/MS/MS scans go one step further than MS/MS scans. A fragment that is produced in the collision cell is fragmented further in the trap to give more structural information about the molecular ion.

Quadrupole-Mode Scan Types

Triple quadrupole instruments have high-sensitivity Multiple Reaction Monitoring (MRM) capabilities required for quantitation experiments. In addition, they have highly specific scan types, such as precursor ion and neutral loss scans, that allow a more advanced search to be performed on the components of the samples.

Q1 MS (Q1): A full scan using the first quadrupole (Q1). The ion intensity is returned for every mass in the scan range.

Q1 Multiple Ions (Q1 MI): A zero width scan type using the Q1 quadrupole. The ion intensity is returned for the specified masses only.

Q3 MS (Q3): A full scan using the third quadrupole (Q3). The ion intensity is returned for every mass in the scan range.

Q3 Multiple Ions (Q3 MI): A zero width scan type using the Q3 quadrupole. The ion intensity is returned for the specified masses only.

MRM (MRM): An MS/MS scan in which a user-selected ion is passed through the Q1 quadrupole and fragmented in the Q2 collision cell. The Q3 quadrupole is then used to specify which fragment ion enters the detector. This scan mode is used primarily for quantitation.

Product Ion (MS2): An MS/MS full scan where the Q1 quadrupole is fixed to transmit a specific precursor ion and the Q3 quadrupole scans a defined mass range. Used to identify all of the products of a particular precursor ion.

Precursor Ion (Prec): An MS/MS scan where the Q3 quadrupole is fixed at a specified mass-to-charge ratio to transmit a specific product ion and the Q1 quadrupole scans a mass range. Used to confirm the presence of a precursor ion or more commonly used to identify compounds sharing a common product ion.

Neutral Loss (NL): An MS/MS scan where both the Q1 quadrupole and the Q3 quadrupole scan a mass range, a fixed mass apart. A response is observed if the ion chosen by the first analyzer fragments by losing the neutral loss (the fixed mass) specified. Used to confirm the presence of a precursor ion or more commonly used to identify compounds sharing a common neutral loss.

LIT-Mode Scan Types

The LIT-mode scans use the Q3 quadrupole as a linear ion trap. Ions are trapped and stored in the trap before being scanned out, giving increased sensitivity. In addition, MS/MS/MS analysis can be performed in the linear ion trap, providing more information about the sample.

Enhanced MS (EMS): Ions are scanned in the Q1 quadrupole to the linear ion trap where they are collected. These ions are scanned out of the Q3 quadrupole to produce single MS type spectra.

Enhanced Multi-Charge (EMC): This scan is similar to the EMS scan except that before scanning the ions out of the linear ion trap, there is a delay period during which low-charge state ions (primarily singly-charged ions) are allowed to preferentially escape from the linear ion trap. When the retained ions are scanned out, the multiply-charged ion population dominates the resulting spectrum.

Enhanced Product Ion (EPI): This scan type is used to obtain a high quality MS/MS spectrum on a specific ion. The fragmentation is done in the Q2 collision cell and thus provides the information-rich MS/MS spectrum typical of collisionally activated dissociation fragmentation. In this scan mode, the precursor ion to be fragmented is first selected in the Q1 quadrupole with a mass window that is 1 to 4 Da wide, filtering out all other ions. The precursor ion is fragmented by collisionally activated dissociation (CAD) gas in the Q2 collision cell. The fragment ions generated are captured in the linear ion trap and then scanned out at one of three scan speeds, depending on the required fragment ion resolution.

For IDA experiments, the **Product Of** field is set to 30 Da by default, and this value should not be changed.

Enhanced Resolution (ER): This scan is similar to the EMS scan except that a small 30 Da mass around the precursor mass is scanned out of the linear ion trap at the slowest scan rate to produce a narrow window of the best-resolved spectra.

MS/MS/MS (MS3): In this scan mode, a precursor ion is selected by the Q1 quadrupole and fragmented with collisionally activated dissociation in the Q2 collision cell. The resulting product ions are all transmitted to the linear ion trap, where a single product ion is then isolated. The isolated ion is further fragmented in the linear ion trap, and the resulting product ions are scanned out of the ion trap at one of three scan speeds. As with any in-trap Collision Induced Disassociation (CID) technique, there is a low mass cut-off for the second MS/MS step due to the condition that the lowest mass fragment and precursor must be simultaneously stable in the trap. For QTRAP® systems, this results in the loss of ions lower than 28 percent of the mass of the precursor ion during MS3 experiments. This phenomenon is often referred to as the one-third cut-off rule.

About Spectral Data Acquisition

Spectral data can be acquired in one of three modes, as shown in the following table.

Table 8-1 Spectral Data Acquisition

Mode	Description
Profile	The preset value is 0.1 Da. Profile data is the data generated by the mass spectrometer and corresponds to the intensity recorded at a series of evenly spaced discrete mass values. For example, for a mass range 100 Da to 200 Da and step size 0.1, the mass spectrometer scans 99.95 to 100.05 (records as value 100), 100.05 to 101.15 (records as value 101)…199.95 to 200.05 (records as value 200).
Peak Hopping	The preset value is 1.0 Da. Peak Hopping is a mode of operating a mass spectrometer in which large steps (approximately 1 Da) are made. It has the advantage of speed (fewer data steps are made) but with the loss of peak shape information.
Centroid	The mass spectrometer scans as in profile mode, but creates a centroid of the data, replacing found peaks with the intensity-weighted center of gravity for each peak. Centroid data has the advantage of significantly reducing file size. The disadvantage is that peak shape information is lost, and if data has been collected as a centroid it cannot be altered. We recommend the use of profile mode and centroiding of the data post-acquisition.

Parameters

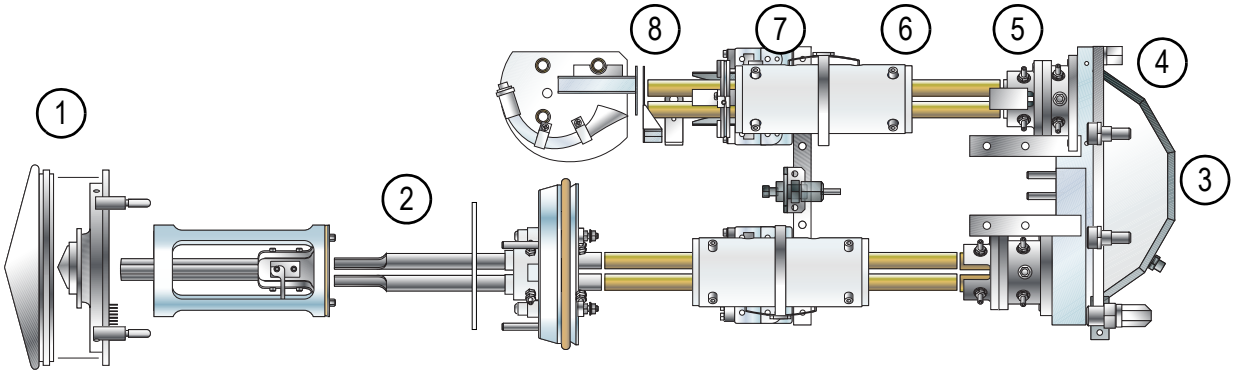
The working parameters are the set of instrument parameters currently being used.

- Source and gas parameters (these parameters can change depending on the ion source used)
- Compound parameters
- Resolution parameters
- Detector parameters

For more information about instrument parameter values and ranges, refer to Appendix A: Parameters for 6500 Series Instruments.

Figure 8-1 shows the location of the parameters on the ion optics path.

Figure 8-1 Ion Optics Path and Parameters



Item	Parameter	Parameter Type	Use	Scan Type
1	IS (IonSpray Voltage)	Source and gas	The IS parameter controls the voltage applied to the electrode that ionizes the sample in the ion source. It depends on the polarity and it affects the spray stability and the sensitivity. This parameter can be compound-dependent and should be optimized for each compound.	All
1	NC (Nebulizer Current)	Source and gas	The NC parameter controls the current applied to the corona discharge needle in the APCI probe, used in the Turbo V™ ion source. The discharge ionizes solvent molecules, which in turn ionize the sample molecules.	All
1	ihe (Interface Heater)	Source and gas	The ihe parameter turns the interface heater on and off. Heating the interface helps maximize the ion signal and prevents contamination of the ion optics. The interface heater should always be on. The button controlling the interface heater reads ON when the interface heater is on.	All
1	IHT (Interface Heater Temperature)	Source and gas	The IHT parameter controls the temperature of the NanoSpray® interface heater and is only available if the NanoSpray ion source and interface are installed.	All
1	sdp	Source and gas	The sdp parameter controls the selection of the DuoSpray™ ion source probes: TurboIonSpray® probe or APCI probe.	n/a

Item	Parameter	Parameter Type	Use	Scan Type
1	DP (Declustering Potential)	Compound	The DP parameter controls the voltage on the orifice, which controls the ability to decluster ions between the orifice and the skimmer (or for systems with an IonDrive QJet® ion guide, between the orifice and IonDrive QJet ion guide). It is used to minimize the solvent clusters that may remain on the sample ions after they enter the vacuum chamber, and, if required, to fragment ions. The higher the voltage, the higher the energy imparted to the ions. If the DP parameter is too high, unwanted fragmentation may occur. Use the preset value and optimize for the compound.	All
1	CUR (Curtain Gas)	Source and gas	The CUR parameter controls the gas flow of the Curtain Gas™ interface. The Curtain Gas interface is located between the curtain plate and the orifice. It assists in solvent evaporation and prevents solvent droplets from entering and contaminating the ion optics. The gas flow should be maintained as high as possible without losing sensitivity.	All
1	GS1 (Gas 1)	Source and gas	The GS1 parameter controls the nebulizer gas. The nebulizer gas helps generate small droplets of sample flow and affects spray stability and sensitivity.	All
1	GS2 (Gas 2)	Source and gas	The GS2 parameter controls the auxiliary, or turbo, gas. It is used to help evaporate the solvent to produce gas phase sample ions.	All
1	TEM (Temperature)	Source and gas	The TEM parameter controls the temperature of the turbo gas (GS2) in the TurboIonSpray probe or the temperature of the probe in the heated nebulizer (or APCI) probe.	All
1	IS (Ion Transfer Voltage)	Source and gas	For the PhotoSpray® ion source, the IS parameter controls the voltage that transfers the ions from the primary ionization region towards the curtain plate orifice.	All

Item	Parameter	Parameter Type	Use	Scan Type
2	EP (Entrance Potential)	Compound	The EP parameter controls the potential difference between the voltage on Q0 and ground. The entrance potential guides and focuses the ions through the high-pressure Q0 region. Use the preset value.	All
2	Q0 Trapping	Compound	The Q0 trapping parameter controls the storage of ions in the Q0 region. It is used to increase sensitivity and duty cycle by trapping ions in the Q0 region while ions are being mass-selectively ejected from the LIT. Use fixed fill time with this parameter. Either select or clear the feature based on the experiment. The recommended fixed fill time to use with Q0 trapping is 20 ms or greater.	EMS, EMC, EPI, ER, and MS/MS/MS,
3	CAD Gas	Source and gas	The CAD parameter controls the pressure of collision gas in the collision cell during Q3, MS/MS-type, and LIT scans. For Q3 scans, the collision gas helps to focus the ions as they pass through the collision cell. The preset for the CAD parameter is in fixed mode. For MS/MS-type scans, the collision gas aids in fragmenting the precursor ions. When the precursor ions collide with the collision gas, they can dissociate to form product ions. For LIT scans, the collision gas helps to focus and trap ions in the LIT. Use the preset value and optimize for the compound.	Q3 MI, Q3 MS, MRM, Prec, NL, EMS, ER, EPI, MS/MS/MS, EMC, and TDF

Item	Parameter	Parameter Type	Use	Scan Type
3	CE (Collision Energy)	Compound	The CE parameter controls the potential difference between Q0 and Q2 (collision cell). It is used only in MS/MS-type scans. This parameter is the amount of energy that the precursor ions receive as they are accelerated into the collision cell, where they collide with gas molecules and fragment. Use the preset value and optimize for the compound.	MRM, MS2, Prec, NL, and LIT
3	CES (Collision Energy Spread)	Compound	The CES parameter, in conjunction with the Collision Energy (CE), determines which three discreet collision energies are applied to the precursor mass in an Enhanced Product Ion (EPI) or MS/MS/MS (MS3) experiment when CES is used. When a collision energy spread value is entered, CES is automatically turned on. Use the preset value and optimize for the compound.	EPI and MS/MS/MS
4	CXP (Collision Cell Exit Potential)	Compound	The CXP parameter is only used in Q3 and MS/MS-type scans, where it transmits the ions into Q3. Use the preset value and optimize for the compound.	Q3, MRM, MS2, Prec, and NL
4	TDF CE (Time Delayed Fragmentation Collision Energy)	Compound	This is the amount of energy that the precursor ions receive as they are accelerated into Q3, where they collide with gas molecules and fragment. Use the preset value.	TDF
5	Q3 Entry Barrier	Compound	The Q3 Entry Barrier parameter is used to transfer the ions from Q2 into the LIT. Use the preset value.	EMS, EMC, EPI, ER, and MS/MS/MS
5	Q3 Empty Time	Compound	The Q3 Empty Time parameter controls the amount of time that singly-charged ions are removed from the LIT. Use the preset value.	EMC

Item	Parameter	Parameter Type	Use	Scan Type
6	MCS (Multi-Charge Separation) Barrier	Compound	The MCS Barrier parameter controls the voltage used to eliminate the singly-charged ions from the LIT. Use the preset value.	EMC
6	Q3 Cool Time	Compound	The Q3 Cool Time parameter controls the amount of time that the precursor ions are allowed to cool prior to collection of their product ions. Use the preset value.	TDF
7	MS/MS/MS Fragmentation Time	Compound	The MS/MS/MS Fragmentation Time parameter controls the amount of time that the excitation energy is applied. It is used in combination with the excitation energy to fragment the isolated second precursor ion. Use the preset value.	MS/MS/MS
7	Fixed LIT Fill Time	Compound	The Fixed LIT Fill Time parameter controls the amount of time that the LIT fills with ions. Use the preset value.	EMS, EPI, MRM, and MS/MS/MS
7	DFT (Dynamic Fill Time)	Compound	DFT dynamically calculates the length of time that ions are collected in the LIT based on the incoming ion signal. When DFT is turned on the signal is optimized to either increase sensitivity or minimize space-charging. Either select or clear the feature based on the experiment. In the **Tools > Settings > Method Options** dialog, the Dynamic Fill Time settings are optimized for the 10 000 Da/s scan speed. These settings are also suitable for other LIT scan speeds.	EMS, EPI, ER, and MS/MS/MS
8	EX2	Detector	The second exit lens (EX2) shields the LIT from the high voltage on the detector. The EX2 parameter controls the voltage applied to the LIT. This parameter does not need to be optimized, and by default is set to a fixed value and is not displayed in the Analyst software interface.	Q1, Q3, MS/MS, LIT

Item	Parameter	Parameter Type	Use	Scan Type
8	CEM (CEM)	Detector	The CEM parameter controls the voltage applied to the detector. The voltage controls the detector response.	All

Acquisition Method Editor Icons

Table 8-2 Acquisition Method Editor Icons

Icon	Name	Function
	Mass Spec	Shows the **MS** tab in the **Acquisition Method** editor.
	Period	Right-click to add an experiment, add an **IDA Criteria Level**, or delete the period.
	Autosampler	Opens the **Autosampler Properties** tab.
	Syringe Pump	Opens the **Syringe Pump Properties** tab.
	Column Oven	Opens the **Column Oven Properties** tab.
	Valve	Opens the **Valve Properties** tab.
	DAD	Opens the **DAD Method** Editor. Refer to Show DAD Data on page 88.
	ADC	Opens the **ADC Properties** tab. Refer to Show ADC Data on page 82.

A batch is a collection of information about the samples to be analyzed. Batches tell the software the order in which to analyze the samples. For information about importing batches, refer to the *Advanced User Guide*.

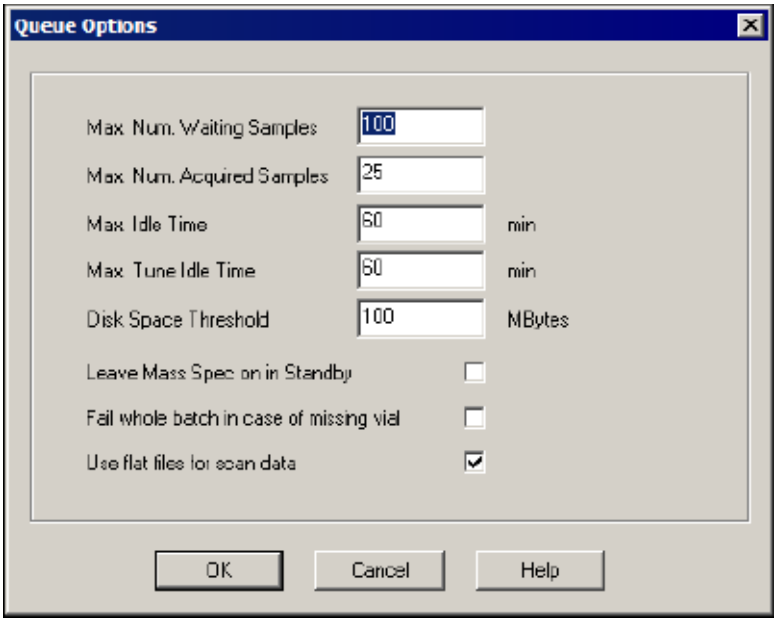
Set Queue Options

The queue goes one by one through the list, acquiring each sample with the selected acquisition method. After all the samples have been acquired, the queue stops and the mass spectrometer goes into the standby mode. In the standby mode, the LC pumps and some instrument voltages are turned off.

The user can change the length of time the queue runs after the last acquisition has finished, before the Analyst software puts the mass spectrometer into the standby mode. For more information about the other fields in the **Queue Options** dialog, refer to the Help.

1. In the navigation bar, click **Configure**.
2. Click **Tools > Settings > Queue Options**.

Figure 9-1 Queue Options Dialog



3. In the **Max Num Waiting Samples** field, set the maximum number of samples to a value that is greater than the number of samples that will be submitted to the queue.
4. In the **Max Idle Time** field, type the length of time the queue will wait after acquisition is completed before going into Standby mode. The preset value is 60 minutes.

   If gas cylinders are used, adjust this time to make sure that the gas in the cylinders is not depleted.

If an LC method is used, then before the run is started, make sure that there is enough solvent in the reservoirs for the primary flow rate for all of the sample runs and the maximum idle time.

5. Select **Leave Mass Spec on in Standby** to keep the mass spectrometer running after analysis has been completed. This feature allows the heaters and gases to continue running, even after devices have entered idle state, so that the ion source and entrance to the mass spectrometer are kept free of contaminants.
6. Select **Fail Whole Batch in Case of Missing Vial** to fail the entire batch when a missing vial is encountered. If this option is not selected, only the current sample will fail and the queue will continue to the next sample.

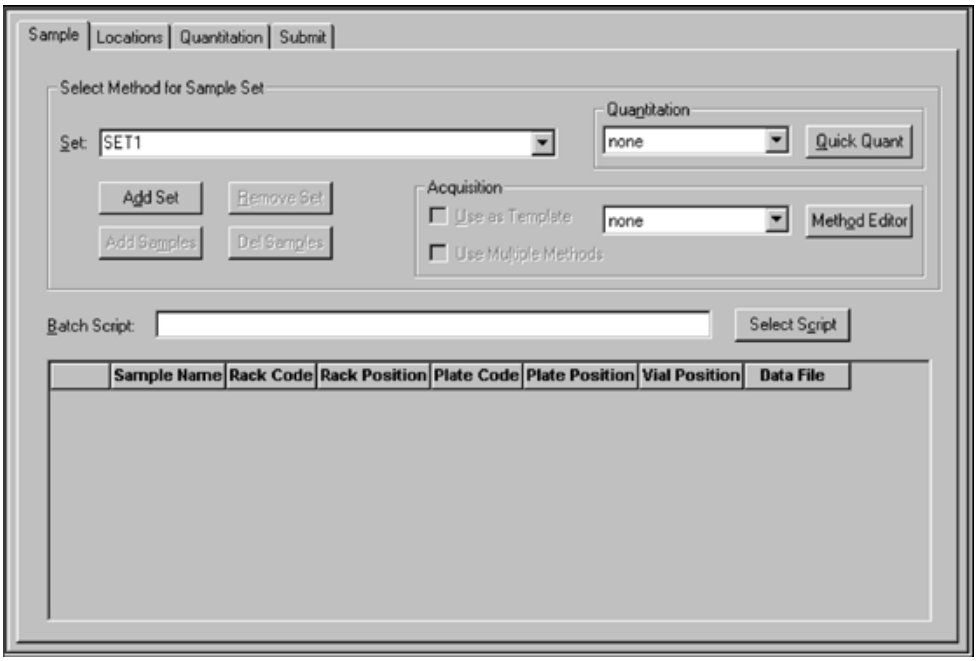
Add Sets and Samples to a Batch

A set can consist of a single sample or multiple samples.

Note: For more information about adding quantitation information to a batch, refer to the *Advanced User Guide*.

1. In the navigation bar, under **Acquire**, double-click **Build Acquisition Batch**.

Figure 9-2 Batch Editor Dialog



2. In the **Sample** tab, in the **Set** list, type a name.
3. Click **Add Set**.
4. Click **Add Samples** to add samples to the new set.
5. In the **Sample name** section, in the **Prefix** field, type a name for the samples in this set.

6. To add incremental numbering to the end of the sample name, select the **Sample number** check box.
7. If the **Sample number** check box is selected, in the **Number of digits** field, type the number of digits to include in the sample name.

   For example, if 3 is typed, the sample names would be *samplename*001, *samplename*002, *samplename*003.
8. In the **Data file** section, in the **Prefix** field, type a name for the data file that will store the sample information.
9. Select the **Set name** check box to use the set name as part of the data file name.
10. Select the **Auto Increment** check box to increment the data file names automatically.
11. In the **Sub Folder** field, type a name.

    The folder is stored in the Data folder for the current project. If the Sub folder field is left blank, the data file is stored in the Data folder and a subfolder is not created.
12. In the **New samples** section, in the **Number** field, type the number of new samples.
13. Click **OK**.

    The sample table fills with the sample names and data file names.

Tip! **Fill Down** and **Auto Increment** options are available in the right-click menu after a single column heading or several rows in a column are selected.

14. In the **Sample** tab, in the **Acquisition** section, select a method from the list.

    Depending on how the system is set up, specific information for the autosampler must be entered. Even if the injection volume is set in the method, the injection volume can be changed for one or more samples by changing the value in the injection volume column.

Tip! To use different methods for some of the samples in this set, select the **Use Multiple Methods** check box. The **Acquisition Method** column is shown in the **Sample** table. Select the acquisition method for each sample in this column.

15. To change the injection volumes from the volumes listed in the method, in the **Inj. Volume (µL)** column, type the injection volume for each sample.
16. In the **Vial Position** column, indicate the positions of the vials.

Tip! To automatically fill in the samples from the **Locations** tab, click on the first and last vial within a set with the **Shift** key held down. These vials appear as red circles. On the **Locations** tab, multiple injections from the same vial can be done by holding down the **Ctrl** key while clicking the vial location. The red circle turns green.

17. To set sample locations, do one of the following:
    - Set Sample Locations in the Batch Editor on page 69

- Select Vial Positions using the Locations Tab (Optional) on page 69

Submit a Sample or Set of Samples

1. In the **Batch Editor**, click the **Submit** tab.
2. If the **Submit Status** section contains a message about the status of the batch, do one of the following:
   - If the message indicates that the batch is ready for submission, proceed to step 3.
   - If the message indicates that the batch is not ready for submission, make the changes as indicated by the message.
3. Click **Submit**.
4. Save the file.

Change Sample Order

The order of the samples can be edited before they are submitted to the Queue.

- On the **Submit** tab, double-click any of the numbers on the far left of the table (a very faint square box is visible), and then drag them to the new location

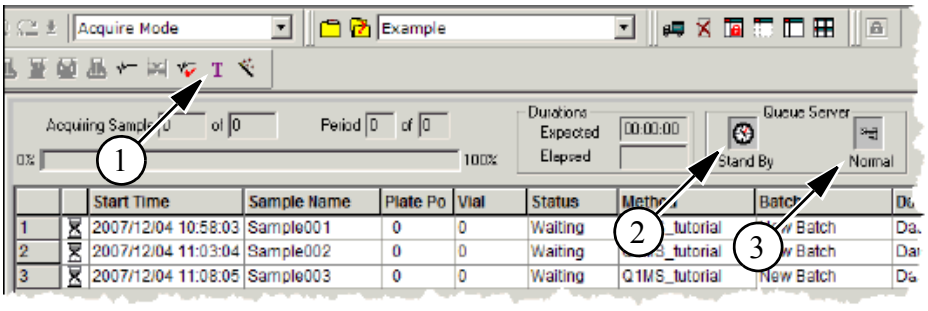
Acquire Data

The system must not be in Tune mode when sample acquisition is started. Also, if the system has been previously run that day and has not yet been set to Standby, sample acquisition will start automatically.

1. In the navigation bar, click **Acquire**.
2. Click **View > Sample Queue**.

   The Queue Manager opens with all submitted samples.

Figure 9-3 Queue Manager



Item	Description
1	The **Reserve Instrument for Tuning** icon should not be pressed in.

Item	Description
2	Queue status should be **Stand By**.
3	Queue Server should be in **Normal** mode. Refer to Queue States on page 73.

3. Click **Acquire > Start Sample**.

Note: It is recommended that the user runs the sample again in the event of an abnormal termination during sample acquisition.

Set Sample Locations in the Batch Editor

If an autosampler is used in the acquisition method, then the vial positions of the samples must be defined in the acquisition batch. Define the location in the **Sample** tab or in the **Locations** tab. For more information about creating batches, refer to Add Sets and Samples to a Batch on page 66.

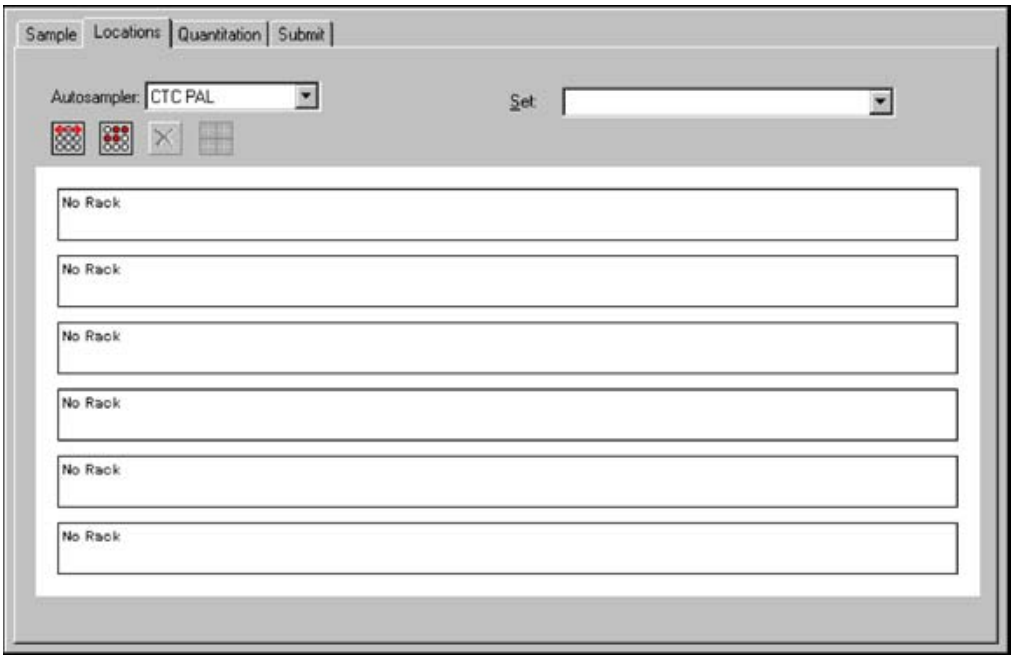
Note: Depending on the autosampler being used, it may not be necessary to type details in additional columns.

1. In the **Sample** tab, in the **Set** list, select the set.
2. For each sample in the set, do the following if applicable:
   - In the **Rack Code** column, select the rack type.
   - In the **Rack Position** column, select the position of the rack in the autosampler.
   - In the **Plate Code** column, select the plate type.
   - In the **Plate Position** column, select the position of the plate on the rack.
   - In the **Vial Position** column, type the position of the vial in the plate or tray.
3. Save the file.

Select Vial Positions using the Locations Tab (Optional)

1. In the **Batch Editor**, click the **Locations** tab.

Figure 9-4 Batch Editor, Locations Tab



2. In the **Set** list, select the set.
3. In the **Autosampler** list, select the autosampler.

   The appropriate number of rack spaces for the autosampler is shown in the graphic rack display.
4. In the space associated with the rack, right-click and then select the rack type.

   The plates or trays are shown in the rack.
5. Double-click one of the rectangles.

   The circles depicting the wells or vials for the plate or tray are shown.
6. To select whether samples are marked by row or column, click **Row/Column Selection**.

   If the button shows a red horizontal line, the **Batch Editor** marks the samples by row. If the button shows a red vertical line, the **Batch Editor** marks the samples by column.
7. Click the sample wells or vials in the order to be analyzed. Click a selected well or vial again to clear it.
8. Save the file.

Tip! To auto fill in the samples, hold down the **Shift** key and then click the first and last vial within a set. To perform multiple injections from the same vial, hold down the **Ctrl** key and then click the vial location. The red circle changes to a green circle.

Stop Sample Acquisition

When a sample acquisition is stopped, the current scan finishes before the acquisition is stopped.

1. In the **Queue Manager**, click the sample in the queue after the point where acquisition should stop.
2. In the navigation bar, click **Acquire**.
3. Click **Acquire > Stop Sample**.

   The queue stops after the current scan in the selected sample is complete. The sample status in the **Queue Manager (Local)** window changes to Terminated, and all other samples following in the queue are Waiting.
4. To continue processing the batch, click **Acquire > Start Sample**.

Batch and Acquisition Method Editor Tips

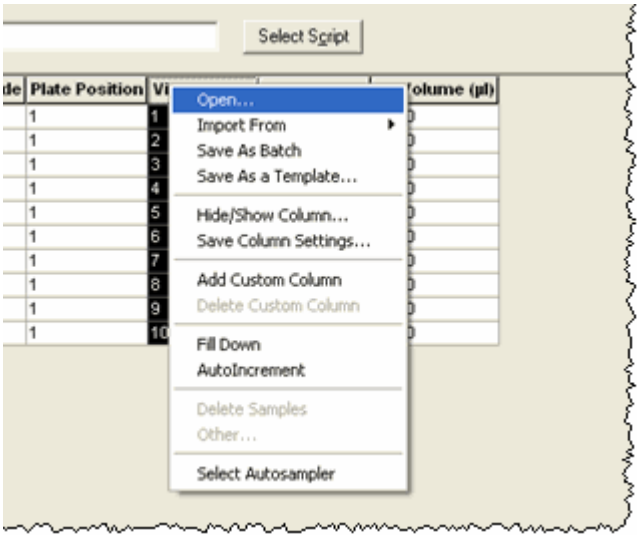
Table 9-1 Tips

To do this...	...do this
To change all the values in a column simultaneously	click a column heading and then right-click. From the menu, use the **Auto Increment** and **Fill Down** commands to change the values in the column. This also works for multiple cells in the same column.
To change an existing acquisition method	from the list, select the method and then click **Method Editor**. To create a new acquisition method, from the list, select **None** and then click **Method Editor**. Only experienced users should use this feature. Do not use this feature if the **Use Multiple Methods** option is used.
To apply a previously created quantitation method	select the method from the **Quantitation** menu.
To select more than one well or vial at a time	hold down the **Shift** key and then click the first and last well or vial in the range.

Batch Editor Right-Click Menu

Right-click in the **Batch Editor** table to access the following options.

Figure 9-5 Batch right-click menu



Menu	Function
Open	Opens a batch file.
Import From	Imports a file.
Save As Batch	Saves the batch with a different name.
Save As a Template	Saves the batch as a template. Used with the Express View feature.
Hide/Show Column	Hides or shows a column.
Save Column Settings	Saves the batch column settings.
Add Custom Column	Adds a custom column.
Delete Custom Column	Deletes a custom column.
Fill Down	Fills the same data into the selected cells.
Auto Increment	Automatically increments data into the selected cells.
Delete Samples	Deletes the selected row.
Select Autosampler	Selects an autosampler.

Queue States and Device Status

The **Queue Manager** shows queue, batch, and sample status. Detailed information about a particular sample in the queue can also be viewed.

Queue States

The current state of the queue is indicated in the **Queue Server**.

Figure 9-6 Queue Server Indicator Showing Normal Mode

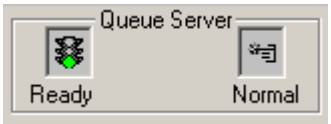
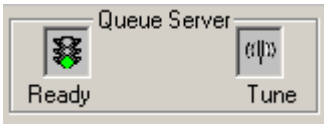


Figure 9-7 Queue Server Indicator Showing Tune Mode



The first icon in Figure 9-6 shows the queue state. The second icon indicates whether the queue is in tune mode (for tuning) or normal mode (for running samples). Table 9-2 shows the various queue states.

Table 9-2 Queue States

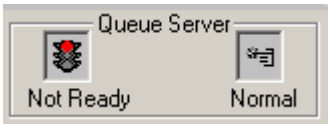
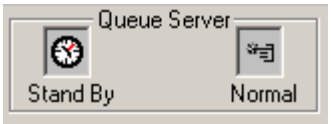
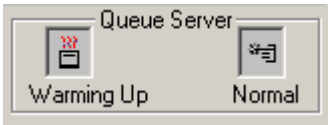
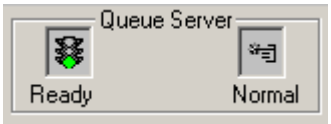
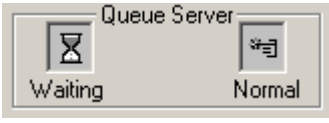
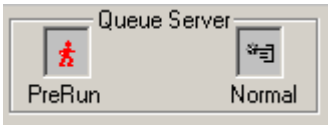
Icons	State	Definition
	Not Ready	In the **Not Ready** state, the hardware profile is deactivated and the queue is not accepting any sample submissions.
	Stand By	In the **Stand By** state, the hardware profile has been activated, but all devices are idle. Pumps are not running and gases are turned off.
	Warming Up	In the **Warming Up** state, the mass spectrometer and devices are equilibrating, columns are being conditioned, the autosampler needle is being washed, and column ovens are reaching temperature. The period of equilibration is selected by the operator. From this state, the system can go to the **Ready** state.
	Ready	In the **Ready** state, the system is ready to start running samples and the devices have been equilibrated and are ready to run. In this state, the queue can receive samples and will run after samples are submitted.
	Waiting	In the **Waiting** state, the system will automatically begin acquisition when the next sample is submitted.

Table 9-2 Queue States (Continued)

Icons	State	Definition
	PreRun	In the **PreRun** state, the method is being downloaded to each device and device equilibration is occurring. This state occurs before the acquisition of each sample in a batch.
	Acquiring	In the **Acquiring** state, the method is run and data acquisition occurs.
	Paused	In the **Paused** state, the system has been paused during acquisition.

View Instrument and Device Status Icons

Icons representing the mass spectrometer and each device in the active hardware configuration are shown on the status bar in the bottom right corner of the window. The user can view the detailed status of an LC pump to check if the LC pump pressure is appropriate, or view the detailed status of the mass spectrometer to check the temperature of the ion source.

- On the status bar, double-click the icon for the device or mass spectrometer.

  The **Instrument Status** dialog opens.

Table 9-3 Instrument and Device Status (showing the instrument icon)

Status	Icon	Background Color	Description
Idle		Green or yellow	The device is not running. If the background color is yellow, the device should be equilibrated before it is ready to run. If the background color is green, the device is ready to run.
Equilibrating		Green or yellow	The device is equilibrating.
Waiting		Green	The device is waiting for a command from the software or another device, or for some action by the operator.
Running		Green	The device is running a batch.

Table 9-3 Instrument and Device Status (showing the instrument icon) (Continued)

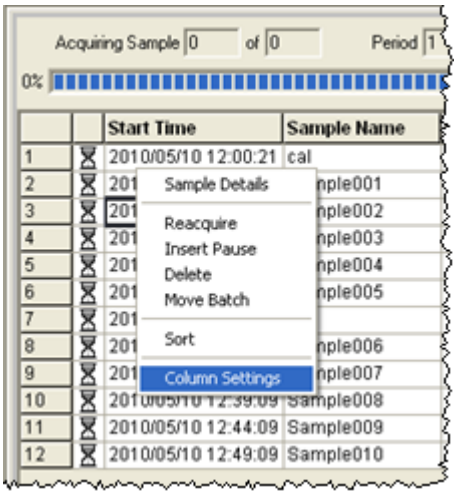
Status	Icon	Background Color	Description
Aborting		Green	The device is aborting a run.
Downloading		Green	A method is being transferred to the device.
Ready		Green	The device is not running, but is ready to run.
Error		Red	The device has encountered an error that should be investigated.

Note: For each status the background color can also be red. This situation means that the device encountered an error while in that status.

Queue Right-Click Menu

Right-click in the Queue table to access the following options.

Figure 9-8 Queue Manager right-click menu



Menu	Function
Sample Details	Opens the **Sample Details** dialog.
Reacquire	Acquires a sample again.
Insert Pause	Inserts a pause, in seconds, between two samples.
Delete	Deletes either the batch or the selected samples.
Move Batch	Moves the batch within the queue.

Menu	Function
Sort	Sorts by the preselect column.
Column Settings	Changes the column settings.

Icon Quick Reference: Acquire Mode

Table 9-4 Acquire Mode Icons

Icon	Name	Function
	View Queue	Shows the sample queue.
	Instrument Queue	Shows a remote instrument station.
	Status for Remote Instrument	Shows the status of a remote instrument.
	Start Sample	Starts the sample in the queue.
	Stop Sample	Stops the sample in the queue.
	Abort Sample	Aborts a sample acquisition in the middle of the processing of that sample.
	Stop Queue	Stops the queue before it has completed processing all the samples.
	Pause Sample Now	Inserts a pause in the queue.
	Insert Pause before Selected Sample	Inserts a pause before a specific sample.
	Continue Sample	Continues acquiring the sample.
	Next Period	Starts a new period.
	Extend Period	Extends the current period.
	Next Sample	Stop acquiring the current sample and starts acquiring the next sample.
	Equilibrate	Selects the method to be used to equilibrate the devices. This method should be the same as the method used with the first sample in the queue.

Table 9-4 Acquire Mode Icons (Continued)

Icon	Name	Function
	Standby	Puts the instrument in standby mode.
	Ready	Puts the instrument in ready mode.
	Reserve Instrument for Tuning	Reserves the instrument for tuning and calibrating.
	IDA Method Wizard	Starts the **IDA Method Wizard**.

Operating Instructions — Analyze and Process Data

10

Use the sample files installed in the Example folder to learn how to view and analyze data using the most common analysis and processing tools. For more information about the following topics, refer to the *Advanced User Guide*.

- Labeling graphs
- Overlaying and summing spectra or chromatograms
- Performing background subtractions
- Smoothing algorithms
- Working with smoothed data
- Working with centroid data
- Working with contour plots
- Working with the fragment interpretation tool
- Working with library databases and library records

Open Data Files

- In the navigation bar, under **Explore**, double-click **Open Data File**.

  The Select Sample dialog opens.

Tip! To see an example data file, make sure that the **Example** project is selected. Open the **Triple Quad** folder, and then open the **QuanData.wiff** file. In the **Sample** list, select **AP13-020**.

The data acquired from the sample is shown. If data is still being acquired, the mass spectrum, DAD/UV trace, and TIC continue to update automatically.

Tip! To turn off the automatic update on the mass spectrum, right-click the mass spectrum and then click **Show Last Scan**. If there is a check mark beside **Show Last Scan**, then the spectrum will update in real time.

Navigate Between Samples in a Data File

Prerequisite Procedure
• Open Data Files on page 79

Note: Table 10-9 shows the navigation icons used in this procedure. If samples were saved in separate data files, then open each file individually.

- To skip to the next sample in the data file, click the icon with the arrow pointing to the right.
- To skip to a non-sequential sample, click the icon with the arrow curving to the right.
- In the **Select Sample** dialog, in the **Sample** list, select the sample.
- To go to the previous sample in the data file, click the icon with the arrow pointing to the left.

Show Experimental Conditions

The experimental conditions used to collect data are stored in the data file with the results. The information contains the details of the acquisition method used: the MS acquisition method (that is, the number of periods, experiments and cycles) including instrument parameters, and HPLC device method (LC pump flow rate). In addition, it also contains the MS resolution and mass calibration tables used for the sample acquisition. Table 10-1 shows the software functionality available when the user views the file information.

Note: If data is acquired from more than one sample into the same .wiff file, the file information pane will not refresh automatically as the user scrolls through the samples. Close the file information pane and then reopen it to view the details for the next sample in the .wiff file.

- Click **Explore** > **Show** > **Show File Information**.

  The File Information pane opens below the graph.

Tip! To create an acquisition method from the file information pane, right-click the file information pane and then click **Save Acquisition Method.**

Table 10-1 Right-Click Menu for Show File Information Pane

Menu	Function
Copy	Copies the selected data.
Paste	Pastes data.
Select All	Selects all the data in the pane.
Save To File	Saves data in an .rtf file.
Font	Changes the font.
Save Acquisition Method	Saves the acquisition method as .dam file.
Save Acquisition Method to CompoundDB	Opens the **Specify Compound Information** dialog. Select the IDs and molecular weights to be saved in the compound database.
Delete Pane	Deletes the pane.

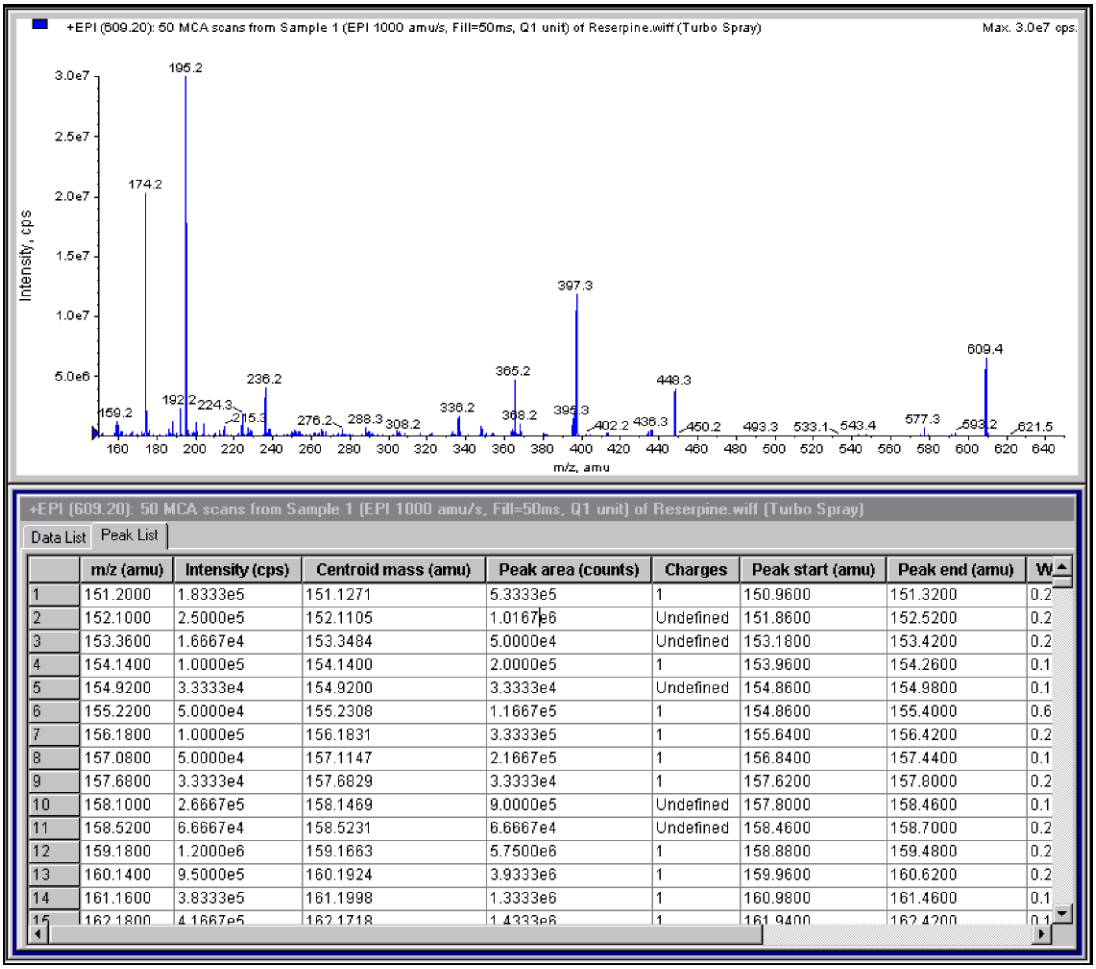
Show Data in Tables

Prerequisite Procedure
• Open Data Files on page 79

- Click **Explore** > **Show** > **Show List Data**.

  The data is shown in a pane below the graph.

Figure 10-1 Peak List Tab


+EPI (609.20): 50 MCA scans from Sample 1 (EPI 1000 amu/s, Fill=50ms, Q1 unit) of Reserpine.wiff (Turbo Spray)
Max. 3.0e7 cps.
Intensity, cps
m/z, amu
+EPI (609.20): 50 MCA scans from Sample 1 (EPI 1000 amu/s, Fill=50ms, Q1 unit) of Reserpine.wiff (Turbo Spray)
Data List
Peak List

	m/z (amu)	Intensity (cps)	Centroid mass (amu)	Peak area (counts)	Charges	Peak start (amu)	Peak end (amu)	W
1	151.2000	1.8333e5	151.1271	5.3333e5	1	150.9600	151.3200	0.2
2	152.1000	2.5000e5	152.1105	1.0167e6	Undefined	151.8600	152.5200	0.2
3	153.3600	1.6667e4	153.3484	5.0000e4	Undefined	153.1800	153.4200	0.2
4	154.1400	1.0000e5	154.1400	2.0000e5	1	153.9600	154.2600	0.1
5	154.9200	3.3333e4	154.9200	3.3333e4	Undefined	154.8600	154.9800	0.1
6	155.2200	5.0000e4	155.2308	1.1667e5	1	154.8600	155.4000	0.6
7	156.1800	1.0000e5	156.1831	3.3333e5	1	155.6400	156.4200	0.2
8	157.0800	5.0000e4	157.1147	2.1667e5	1	156.8400	157.4400	0.1
9	157.6800	3.3333e4	157.6829	3.3333e4	1	157.6200	157.8000	0.2
10	158.1000	2.6667e5	158.1469	9.0000e5	Undefined	157.8000	158.4600	0.1
11	158.5200	6.6667e4	158.5231	6.6667e4	Undefined	158.4600	158.7000	0.2
12	159.1800	1.2000e6	159.1663	5.7500e6	1	158.8800	159.4800	0.2
13	160.1400	9.5000e5	160.1924	3.9333e6	1	159.9600	160.6200	0.2
14	161.1600	3.8333e5	161.1998	1.3333e6	1	160.9800	161.4600	0.1
15	162.1800	4.1667e5	162.1718	1.4333e6	1	161.9400	162.4200	0.1

Table 10-2 RIght-Click Menu for the Spectral Peak List Tab

Menu	Function
Column Options	Opens the Select Columns for Peak List dialog.
Save As Text	Saves the data as text file.
Delete Pane	Deletes the pane.

Table 10-3 Right-Click Menu for the Chromatographic Peak List Tab

Menu	Function
Analyst Classic Parameters	Opens the Analyst Classic dialog.
IntelliQuan Parameters	Opens the Intelliquan dialog.
Save As Text	Saves the data as text file.
Delete Pane	Deletes the pane.

Show ADC Data

ADC (analog-to-digital converter) data is acquired from a secondary detector (for example from a UV detector through an ADC card), and is useful for comparison with mass spectrometer data. To make ADC data available, acquire the data and the mass spectrometer data simultaneously and save it in the same file.

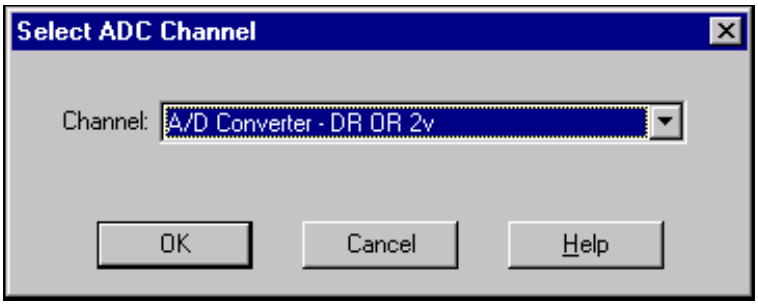
Prerequisite Procedure
• Open Data Files on page 79. Open a data file containing ADC data.

Tip! To see an example ADC data file, make sure that the **Example** project is selected. Open the **Devices** folder, and then open the **Adc16chan.wiff** file.

1. Click **Explore > Show > Show ADC Data**.

   The **Select ADC Channel** dialog opens.

Figure 10-2 Select ADC Channel Dialog



2. In the **Channel** list, select a channel.
3. Click **OK**.

   The ADC data opens in a new pane below the active pane.

Show Basic Quantitative Data

Prerequisite Procedure
• Open Data Files on page 79

1. In the **Peak List** tab, right-click and select **Show Peaks in Graph.**

   Peaks are shown in two colors.

2. To change the peak finding algorithm settings, right-click and then select either **Analyst Classic Parameters** or **Intelliquan Parameters**, which ever is active.
3. (Optional) To remove the colored peaks, right-click in the **Peak List** tab and then clear **Show Peaks in Graph**.

Chromatograms

Table 10-4 Chromatograms

Types of Chromatograms	Purpose
TIC (Total Ion Chromatogram)	A chromatographic display generated by plotting the intensity of all ions in a scan against time or scan number. When a data file is opened, it is preset to appear as a TIC. If the experiment contains only one scan, it is shown as a spectrum. For more information about using the available icons, refer to Table 10-8. If the **MCA** check box is selected during acquisition of the data file, then the data file opens to the mass spectrum. If the **MCA** check box is not selected, then the data file opens with the TIC.
XIC (Extracted Ion Chromatogram)	An ion chromatogram created by taking intensity values at a single, discrete mass value, or a mass range, from a series of mass spectral scans. It indicates the behavior of a given mass, or mass range, as a function of time.
BPC (Base Peak Chromatogram)	A chromatographic plot that shows the intensity of the most intense ion within a scan versus time or scan number.
TWC (Total Wavelength Chromatogram)	A chromatographic display created by summing all of the absorbance values in the acquired wavelength range and then plotting the values against time. It consists of the summed absorbances of all ions in a scan plotted against time in a chromatographic pane.
XWC (Extracted Wavelength Chromatogram)	A subset of TWC. An XWC shows the absorbance for a single wavelength or the sum of the absorbance for a range of wavelengths.
DAD (Diode Array Detector)	A UV detector that monitors the absorption spectrum of eluting compounds at one or more wavelengths.

Show TICs from a Spectrum

Prerequisite Procedure
• Open Data Files on page 79. Open a data file containing spectra.

Tip! To see an example data file, make sure that the Example project is selected. Open the LIT folder, and then open the Reserpine.wiff file.

- Click **Explore > Show > Show TIC**.

  The TIC opens in a new pane.

  Tip! Right-click inside a pane containing a spectrum and then click **Show TIC**.

Show a Spectrum from a TIC

1. In a pane containing a TIC, select a range.
2. Click **Explore > Show > Show Spectrum**.

   The spectrum opens in a new pane.

   Tip! Double-click in the TIC pane at a particular time to show the spectrum.

Generate XICs

XICs can be generated only from single period, single experiment chromatograms or spectra. To obtain an XIC from multi-period or multi-experiment data, split the data into separate panes by clicking the triangle under the x-axis. For more information about using the available icons, refer to Table 10-8.

Several methods are available for extracting ions to generate an XIC, depending on whether chromatographic or spectral data is used. Table 10-5 contains a summary of methods that can be used with chromatograms and spectra.

Table 10-5 Summary of XIC Generation Methods

Method	Use with Chromatogram	Use with Spectrum	Extraction
Selected range	No	Yes	Extracts ions from a selected area in a spectrum.
Maximum	No	Yes	Extracts ions from a selected area in a spectrum using the most intense peak in the selected area. This option creates an XIC using the maximum mass from the selected spectral range.

Table 10-5 Summary of XIC Generation Methods (Continued)

Method	Use with Chromatogram	Use with Spectrum	Extraction
Base peak masses	Yes	No	Can be used only with BPCs (Base Peak Chromatograms.) Use the **Use Base Peak Masses** command to extract ions results in an XIC with a different colored trace for each mass. If the selection includes multiple peaks, the resulting XIC will have an equal number of colored traces representing each mass.
Specified masses	Yes	Yes	Extracts ions from any type of spectrum or chromatogram. Select up to ten start and stop masses for which to generate XICs.

Prerequisite Procedure
• Open Data Files on page 79. Open a data file containing spectra.

Tip! To see an example data file, make sure that the **Example** project is selected. Open the **LIT** folder, and then open the **Reserpine.wiff** file.

Generate an XIC Using a Selected Range

1. Select a range by clicking and holding the left mouse button at the start of the range and then dragging the cursor to the stop point and release.

   The selection is highlighted in blue.

2. Click **Explore > Extract Ions > Use Range**.

   An XIC of the specified selection opens in a pane below the spectrum pane. The experiment information at the top of the pane contains the mass range and the maximum intensity in counts per second.

Generate an XIC Using the Maximum Peak

1. Select a range.

   The selection is highlighted in blue.

2. Click **Explore > Extract Ions** > **Use Maximum**.

   An XIC of the maximum peak specified selection opens below the spectrum pane. The experiment information at the top of the pane contains the mass range and the maximum intensity in counts per second.

Generate an XIC Using Base Peak Masses

1. In a BPC, select the peak from which to extract ions.

   The selection is highlighted in blue.

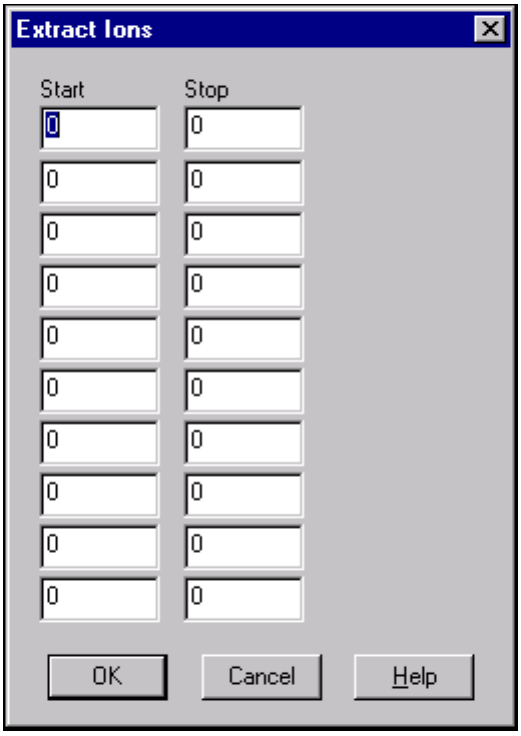
2. Click **Explore > Extract Ions** > **Use Base Peak Masses**.

   An XIC of the specified selection opens below the spectrum pane. The experiment information at the top of the pane shows the mass range and the maximum intensity in counts per second.

Extract Ions by Selecting Masses

1. Open a spectrum or chromatogram.
2. Click **Explore > Extract Ions** > **Use Dialog**.

Figure 10-3 Extract Ions Dialog



3. Type the values for each XIC to be created. If a stop value is not typed, then the range is defined by the start value.
   - In the **Start** field, type the start value (lower value) for the mass range.
   - In the **Stop** field, type the stop value (higher value) for the mass range.
4. Click **OK**.

   An XIC of the selection opens below the chromatogram pane. The experiment information at the top of the pane includes the masses and the maximum intensity in counts per second.

Generate BPCs

BPCs can be generated only from single period, single experiment data. For more information about using the available icons, refer to Table 10-8.

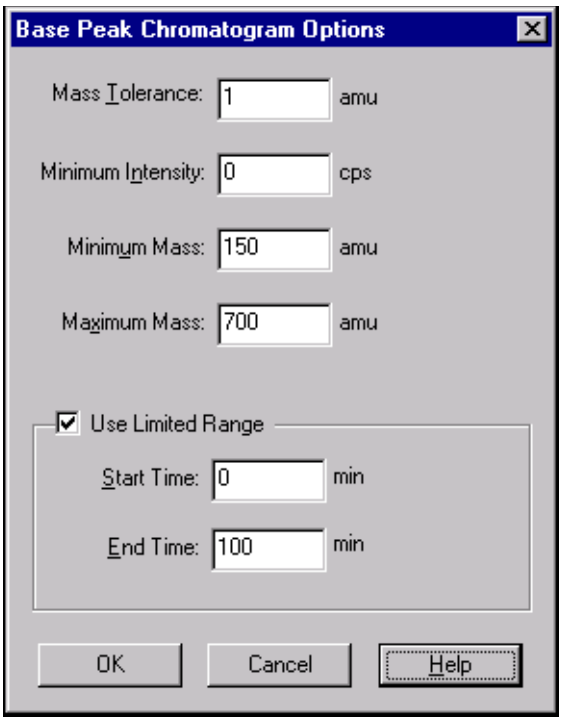
1. Select an area within a TIC.

The selection is highlighted in blue.

2. Click **Explore > Show > Show Base Peak Chromatogram**.

   The selections are shown in the **Start Time** and **End Time** fields.

Figure 10-4 Base Peak Chromatogram Options Dialog



3. In the **Mass Tolerance** field, type the value to dictate the mass range used to find a peak. The software finds the peak using a value twice the typed range (± the mass value).
4. In the **Minimum Intensity** field, type the intensity below which peaks are ignored by the algorithm.
5. In the **Minimum Mass** field, type the mass that determines the beginning of the scan range.
6. In the **Maximum Mass** field, type the mass that determines the end of the scan range.
7. To set the start and end times, select the **Use Limited Range** check box and do the following:
   - In the **Start Time** field, type the time that determines the start of the experiment.
   - In the **End Time** field, type the time that determines the end of the experiment.
8. Click **OK**.

   The BPC is generated in a new pane.

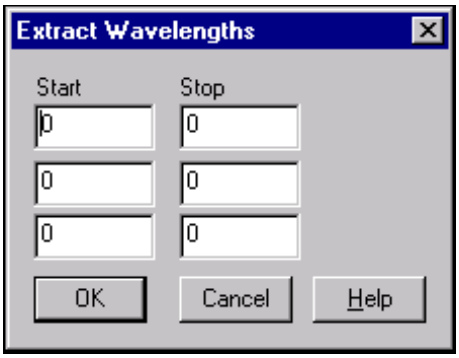
Generate XWCs

Up to three ranges can be extracted from a DAD spectrum to generate the XWC. For more information about using the available icons, refer to Table 10-8.

Prerequisite Procedure
• Open Data Files on page 79. Open a data file that contains a DAD spectrum.

1. Anywhere in the pane, right-click and then click **Extract Wavelengths**.

Figure 10-5 Extract Wavelengths Dialog



2. Type start and stop values.
3. Click **OK**.

   The XWC opens in a pane below the DAD spectrum.

Show DAD Data

Like mass spectrometer data, DAD data can be viewed in chromatogram or spectrum form.

Prerequisite Procedure
• Open Data Files on page 79. Open a data file containing data acquired with a DAD. The TWC, which is analogous to a TIC, opens in a pane below the TIC.

1. In the TWC pane, click a point to select a single point in time, or highlight an area of the spectrum to select a range of time.
2. Click **Explore > Show > Show DAD Spectrum**.

   The DAD spectrum opens in a pane below the TWC. The y-axis shows absorbance and the x-axis shows wavelength.

Tip! If the pane with the TWC is closed, click a point anywhere in the TWC to open it again. Click **Explore** > **Show** > **Show DAD TWC**.

Generate TWCs

A TWC shows total absorbance (mAU) on the y-axis plotted against time on the x-axis. For more information about using the available icons, refer to Table 10-8.

Prerequisite Procedure
• Open Data Files on page 79. Open a data file that contains a DAD spectrum.

- Click **Explore > Show > Show DAD TWC**.

  The TWC opens in a pane below the DAD spectrum.

Tip! Right-click inside the pane containing the DAD spectrum and then click **Show DAD TWC**.

Adjust the Threshold

The threshold is an invisible line drawn parallel to the x-axis of a graph that sets a limit below which the software will not include peaks in a spectrum. The line has a handle, represented by a blue triangle to the left of the y-axis. Click the blue triangle to view a dotted line that represents the threshold. The threshold can be raised or lowered, but changing the threshold value does not change the data. The software does not label any peaks in the region that lies below the threshold.

Prerequisite Procedure
• Open Data Files on page 79

- Do one of the following:
  - To raise the threshold, drag the blue triangle up the y-axis. To lower the threshold, drag the blue triangle down.
  - Click **Explore > Set Threshold**. In the **Threshold Options** dialog that opens, type the threshold value.
  - Click **Explore > Threshold**.

  The graph updates to show the new threshold. Peak labeling and the peak list are also updated.

Tip! To view the current threshold value, move the pointer over the threshold handle.

Table 10-6 Right-Click Menu for Chromatogram Panes

Menu	Function
List Data	Lists the data points and integrates the peaks found in chromatograms.
Show Spectrum	Generates a new pane.

Table 10-6 Right-Click Menu for Chromatogram Panes (Continued)

Menu	Function
Show Contour Plot	Shows a color-coded plot of a data set, where the color represents the intensity of the data at that point. Only certain MS modes are supported.
Extract Ions	Extracts a specific ion or set of ions from a selected pane and then generates a new pane containing a chromatograph for the specific ions.
Show Base Peak Chromatogram	Generates a new pane containing a base peak chromatogram.
Show ADC Data	Generates a new pane containing the UV data trace, if acquired.
Spectral Arithmetic Wizard	Opens the Spectral Arithmetic Wizard.
Save to Text File	Generates a text file of the pane, which can be opened in Excel or other programs.
Save Explore History	Saves information about changes to processing parameters, also called **Processing Options**, that were made when a .wiff file was processed in explore mode. The processing history is stored in a file with an .EPH (Explore Processing History) extension.
Add Caption	Adds a caption at the cursor point in the pane.
Add User Text	Adds a text box at the position of the mouse cursor.
Set Subtract Range	Sets the subtract range in the pane.
Clear Subtract Range	Clears the subtract range in the pane.
Subtract Range Locked	Locks or unlocks the subtract ranges. If the subtract ranges are not locked then each subtract range can be moved independently. The subtract ranges are preset to locked.
Delete Pane	Deletes the selected pane.

Table 10-7 Right-Click Menu for Spectra Panes

Menu	Function
List Data	Lists the data points and integrates chromatograms.
Show TIC	Generates a new pane containing the TIC.
Extract Ions	Extracts a specific ion or set of ions from a selected pane and then generates a new pane containing a chromatograph for the specific ions.
Save to Text File	Generates a text file of the pane, which can be opened in Excel or other programs.
Save Explore History	Saves information about changes to processing parameters, also called Processing Options, that were made when a .wiff file was processed in Explore mode. The processing history is stored in a file with an .EPH (Explore Processing History) extension.
Add Caption	Adds a caption at the cursor point in the pane.
Add User Text	Adds a text box at the position of the mouse cursor.

Table 10-7 Right-Click Menu for Spectra Panes (Continued)

Menu	Function
Show Last Scan	Shows the scan prior to the selection.
Select Peaks For Label	In this dialog, select the parameters to reduce peak labeling.
Delete Pane	Deletes the selected pane.
Add a Record	Adds records and compound-related data, including spectra, to the library. An active spectrum is required to perform this task.
Search Library	Searches the library without constraints or with previously saved constraints.
Search With Constraints	Searches the library using the Search Constraints dialog.

Data Processing

Graphical data can be processed many ways. This section provides information and procedures for using some of the most commonly used tools.

The user can zoom in on part of a graph to view a particular peak or an area in greater detail in both spectra and chromatograms. The user can also zoom in repeatedly to view smaller peaks.

Graphs

The same data can be examined in different ways. Data can also be kept for comparison purposes before performing processing operations such as smoothing or subtraction.

A window contains one or more panes arranged in such a way that all the panes are fully visible and they do not overlap.

Panes may be of variable or fixed size. Panes are automatically tiled within the window and are arranged into column and row format. If the size of a window is changed, the panes within the window change in size to accommodate the new size. A window cannot be sized to the point where any of the panes would become smaller than its minimum size.

Two or more windows or panes containing similar data can be linked, for example, spectra with similar mass ranges. As one pane or window is zoomed in, the other pane zooms in simultaneously.

For example, the user can link an XIC to the BPC from which the XIC was extracted. Zooming in the BPC also zooms the XIC, so that both chromatograms show the same magnification.

Table 10-8 Graph Options

To do this...	use this menu option...	...or click this icon
Copy a graph to a new window	• Select the graph to copy. Click **Explore > Duplicate Data** > **In New Window**.	

Table 10-8 Graph Options (Continued)

To do this...	use this menu option...	...or click this icon
Rescale graph to its original size	• Select the graph. Click **Explore > Home Graph**.	

Move a pane	• Select the graph. Click **Window > Move Pane**.
	• Select the pane or window and then drag it to the new position. This position can be within the same window or within another window.
	A four-headed arrow is shown when the cursor is on the boundary of the active window or pane.
	  • If the pane is at the top or bottom of the target pane, the pane moves above or below that pane, respectively.
	  • If the pane is at the left or right of the target pane, the pane moves to the left or right of that pane, respectively.
	  • If the pane is at any other position, the pane moves to the target row. The drop shadow of the pane as the pane is moved around indicates its new position.	

Link panes	1. With the two graphs open, click one to make that pane active. 2. Click **Explore > Link** and then click the other pane.	
Remove linking	• Close one of the panes. Click **Explore > Remove Link**	
Delete a pane	• Select the graph. Click **Window > Delete Pane**.	
Lock a pane	• Select the graph. Click **Window > Lock Panes**.	
Hide a pane	• Select the graph. Click **Window > Hide Pane**.	
Maximize a pane	• Select the graph. Click **Window > Maximize Pane**.	

Table 10-8 Graph Options (Continued)

To do this...	use this menu option...	...or click this icon
Tile panes	• Select the graph. Click **Window > Tile all Panes**.	

Zoom In on the Y-axis

1. Position the pointer to the left of the y-axis and then drag vertically away from the starting point.

   A box is drawn along the y-axis representing the new scale.

Note: Take care when zooming in on the baseline. Zoom in too low and the zoom-in box closes.

2. Release the mouse button to draw the graph to the new scale.

Zoom In on the X-axis

1. Position the pointer under the x-axis to either side of the area to expand and then drag away from the starting point in a horizontal direction to expand the area of interest.
2. Release the mouse button to draw the graph to the new scale.

Tip! To return the graph to the original scale, double-click on either axis. To restore the entire graph to original scale, click **Explore** > **Home Graph**.

Table 10-9 Explore Quick Reference: Chromatograms and Spectrum

Icon	Name	Function
	Open File	Opens files.
	Show Next Sample	Goes to the next sample.
	Show Previous Sample	Goes to the previous sample.
	GoTo Sample	Opens the Select Sample dialog.
	List Data	Views the data in tables.

Table 10-9 Explore Quick Reference: Chromatograms and Spectrum (Continued)

Icon	Name	Function
	Show TIC	Generates a TIC from a spectrum.
	Extract Using Dialog	Extracts ions by selecting masses.
	Show Base Peak Chromatogram	Generates a BPC.
	Show Spectrum	Generates a spectrum from a TIC.
	Copy Graph to new Window	Copies the active graph to a new window.
	Baseline Subtract	Opens the Baseline Subtract dialog.
	Threshold	Adjusts the threshold.
	Noise Filter	Shows the **Noise Filter Options** dialog, which can be used define the minimum width of a peak. Signals below this minimum width are regarded as noise.
	Show ADC	Shows ADC data.
	Show File Info	Shows the experimental conditions used to collect the data.
	Add arrows	Adds arrows to the x-axis of the active graph.
	Remove all arrows	Removes arrows from the x-axis of the active graph.
	Offset Graph	Compensates for slight differences in the time during which the ADC data and the mass spectrometer data were recorded. This is useful when overlaying graphs for comparison.
	Force Peak Labels	Labels all the peaks.
	Expand Selection By	Sets the expansion factor for a portion of a graph to be viewed in greater detail.
	Clear ranges	Returns the expanded selection to normal view.

Table 10-9 Explore Quick Reference: Chromatograms and Spectrum (Continued)

Icon	Name	Function
	Set Selection	Defines start and stop points for a selection. This feature provides more accurate selection than is possible by highlighting the region using the cursor.
	Normalize to Max	Scales a graph to maximum, so that the most intense peak is scaled to full scale, whether or not it is visible.
	Show History	Shows a summary of data processing operations performed on a particular file, such as smoothing, subtraction, calibration, and noise filtering.
	Open Compound Database	Opens the compound database.
	Set Threshold	Adjusts the threshold.
	Show Contour Plot	Shows selected data as either a spectrum graph or an XIC. Additionally, for data acquired by a DAD, a contour plot can show selected data as either a DAD spectrum or an XWC.
	Show DAD TWC	Generates a TWC of the DAD.
	Show DAD	Generates a DAD.
	Extract Wavelength	Extracts up to three wavelength ranges from a DAD spectrum to view the XWC.

Use the sample files found in the **Example** folder to learn how to select samples for quantitation, how to select preset queries and create table-specific queries, and how to analyze the acquired data. For more information about the following topics, refer to the *Advanced User Guide*.

- Metric Plots
- Layout of a Results Table

Quantitative Analysis

Quantitative analysis is used to find the concentration of a particular substance in a sample. By analyzing an unknown sample and comparing it to other samples containing the same substance with known concentrations (standards), the software can calculate the concentration of the unknown sample. The process involves creating a calibration curve using the standards and then calculating the concentration for the unknown sample. The calculated concentrations of each sample are then available in a Results Table.

Quantitation Methods

A quantitation method is a set of parameters used to generate peaks in a sample. The quantitation method can include parameters used to locate and integrate peaks, generate standard curves, and calculate unknown concentrations. A previously saved quantitation method can be selected from the **Quantitation** menu in the batch. For information about creating a batch, refer to Add Sets and Samples to a Batch on page 66.

The user can create a quantitation method before data acquisition and then apply the method to the quantitative data automatically after the batch is complete. Alternatively, a quantitation method can be created and applied post-acquisition.

Three tools can be used to create a quantitation method: the **Quantitation Wizard**, the **Build Quantitation Method**, and **Quick Quant**.

Build Quantitation Method

The **Build Quantitation Method** does not generate a quantitation Results Table although the method can subsequently be used in the **Quantitation Wizard** to create a Results Table. The **Build Quantitation Method** can also be used to change existing quantitation methods. This is the most flexible way of creating a quantitation method.

Quantitation Wizard

With the **Quantitation Wizard**, a Results Table is generated at the same time as the quantitation method. Alternatively, an existing quantitation method can be used to quantitate different sets of data. This is the most common way of creating a quantitation method.

Quick Quant

Quick Quant is part of the **Batch Editor**. Use **Quick Quant** to add compound concentrations prior to data acquisition. Because a sample has not been acquired, a representative sample

cannot be be selected nor can peaks be reviewed. With this process, only the method components are defined.

About Results Tables

Results Tables summarize the calculated concentration of an analyte in each unknown sample based on the calibration curve. Results Tables also include the calibration curves as well as statistics for the results. The user can customize the Results Table and view the Results Tables in layouts.

The data from a Results Table can be exported to a .txt file for use in other applications, such as Microsoft Excel. The user can also export data in the table or just the data in the visible columns.

Quantitation Methods and Results Tables

For the following procedures, use the sample data that is installed with the software. **PK Data** contains the batches **Mix_Batch1** and **Mix_Batch2**. These sample batches are used to demonstrate the usefulness of metric plots to isolate problematic samples. The ions scanned were reserpine (609.4/195.0), minoxidil (210.2/164.2), tolbutamide (271.3/91.1) and rescinnamine (635.4/221.2), which is the internal standard. Batch 1 contains no errors in terms of sample preparation, whereas Batch 2 contains a QC sample where the internal standard was added twice (sample QC2).

Create a Method using the Quantitation Method Editor

Prerequisite Procedures
• Select the **Example** project. Refer to Switch Between Projects and Subprojects on page 48.
• Use the **Analyst Classic** algorithm. Refer to Show Basic Quantitative Data on page 83.

1. In the navigation bar, under **Quantitate**, double-click **Build Quantitation Method**.

   The **Select Sample** dialog opens.
2. In the **Data Files** list, double-click the **Triple Quad** folder.
3. Select **Mix_Batch_2. wiff**.

   The samples in the selected data file are shown in the Samples list.
4. Click **OK**.
5. In the **Internal Standards** table, do the following:
   i. In the **Name** column, select rescinnamine.
   ii. In the **Q1/Q3** column, select 635.400/221.185 for each standard.

   Note: If the **Compound ID** field was populated for the samples and internal standards in the acquisition method, then in the Internal Standards table, when a value in the **Q1/Q3** field is selected, the **Name** field is automatically populated.
6. In the **Analytes** table, do the following:
   i. In the **Name** column, select reserpine.

ii. In the **Internal Standard** column, from the list, select the internal standard to be associated with each analyte.

iii. In the **Q1/Q3** column**,** select 609.400/195.039.

iv. If required, add one or more of the other compounds for a more complex analysis.

Note: If the **Compound ID** field was populated for the samples and internal standards in the acquisition method, then in the Analytes table, the **Name** field and **Q1/Q3** field are populated.

7. Click the **Integration** tab.

   In general, the preset integration parameters are suitable for most peaks.

8. If the integration is not suitable, then change the algorithm.
9. Click the **Show or Hide Parameters** icon to show the additional integration algorithms.
10. Click the **Calibration** tab. The preset parameters are suitable for these samples.
11. Save the quantitation method.

    The new method can be used when a batch is created in the **Batch Editor** or when the **Quantitation Wizard** is used to generate a Results Table.

Note: The quantitation method can only be used in the current project unless it is copied to another project. To do this, click **Tools > Project > Copy Data**. A new project must be created and selected to be available for use.

Create a Results Table using the Quantitation Wizard

Prerequisite Procedures
• Select the **Example** project. Refer to Switch Between Projects and Subprojects on page 48.
• Use the **Analyst Classic** algorithm. Refer to Show Basic Quantitative Data on page 83.

It is recommended that the user validate any queries that are used to analyze data in a Results Table.

1. In the navigation bar, under **Quantitate**, double-click **Quantitation Wizard**.

   The **Create Quantitation Set - Select Samples** page opens.

2. In the **Available Data Files** list, double-click the **Triple Quad** folder.
3. Select **Mix_Batch_2.wiff**.
4. Click **Add All Files**.
5. Click **Next**.

   The **Create Quantitation Set - Select Settings & Query** page opens.

6. In the **Default Query** section, click **Select Existing: Query**.
7. In the **Query** list, select **Accuracy 15%**.

8. Click **Next**.

Note: To create a query at the same time, refer to Create a Standard Query on page 100.

The **Create Quantitation Set - Select Method** page opens.

9. Click **Choose Existing Method**.
10. In the Method list, select **PK Data_Mix.qmf**.
11. Click **Finish**.

The Results Table opens.

Tip! To add or remove samples in the Results Table, click **Tools > Results Table > Add/Remove Samples**.

12. Save the Results Table.

Tip! You can create well-formatted reports from a Results Table using the **Reporter** software. It is recommended that the user validate the results if a **Reporter** template that contains a query is used. Refer to the Reporter chapter.

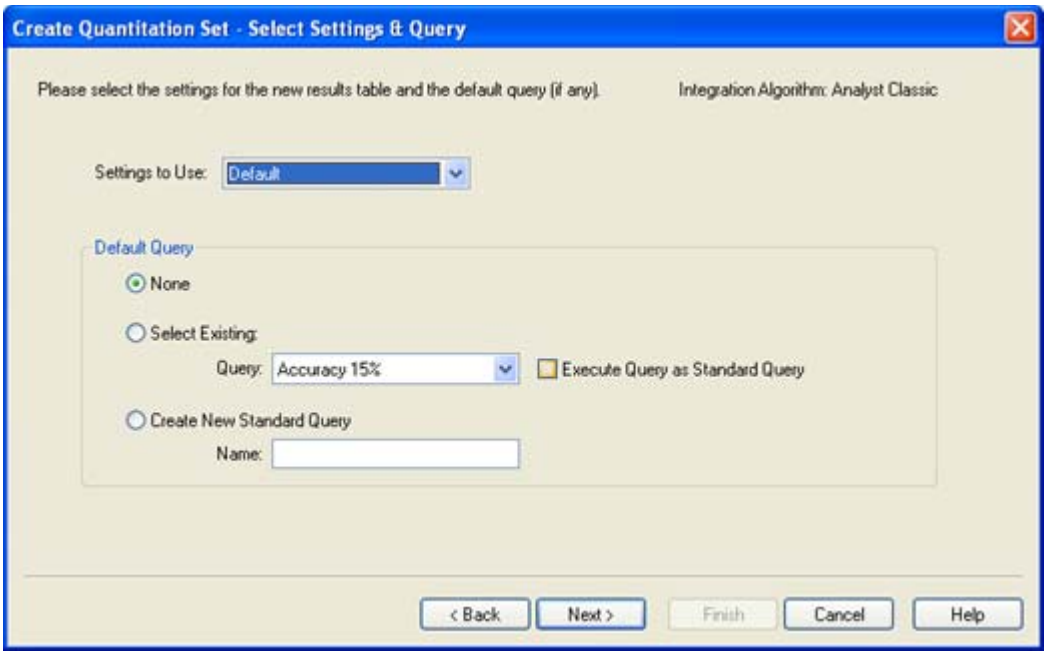
Create a Standard Query

A query and a standard query can be created numerous ways. The following is one example. For more information about creating queries, refer to the Help.

It is recommended that the user validate any queries that are used to analyze data in a Results Table.

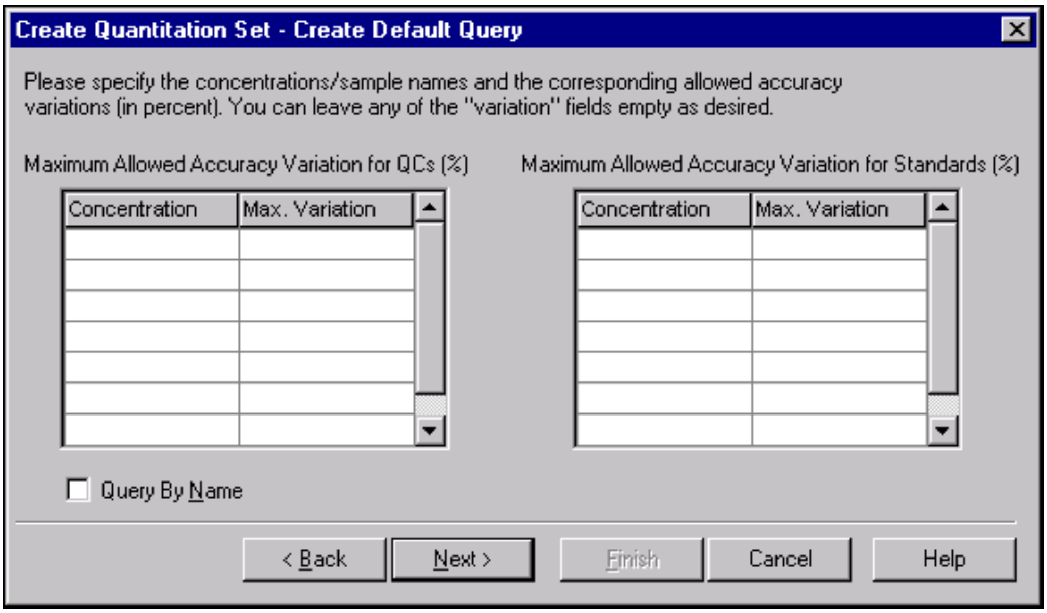
1. In the navigation bar, under **Quantitate**, double-click **Quantitation Wizard**.
2. In the **Create Quantitation Set - Select Samples** page, select samples.
3. Click **Next**.
4. In the **Select Settings & Query** page, in the **Default Query** section, select **Create New Standard Query**.
5. Type a query name.

Figure 11-1 Create Quantitation Set - Select Settings & Query Page



6. Click **Next**.

Figure 11-2 Create Default Query Page

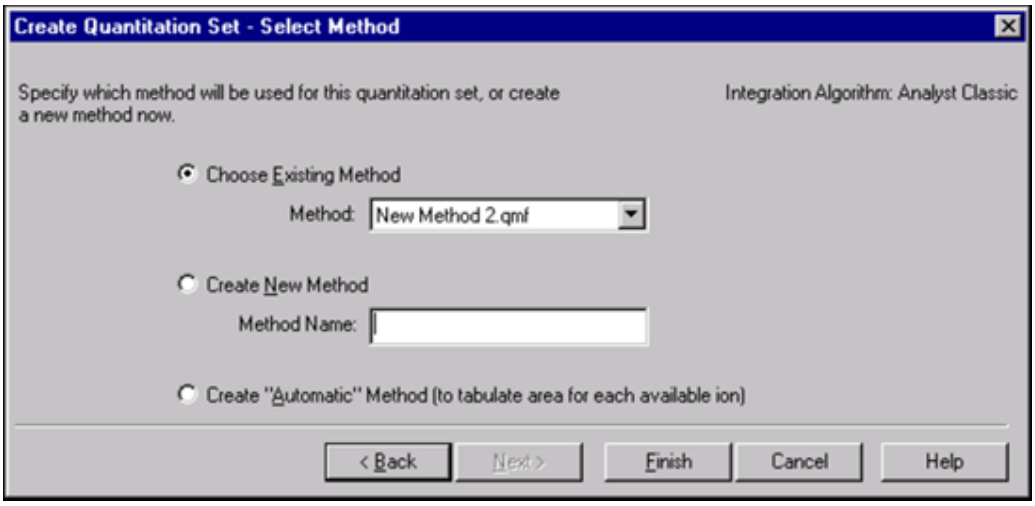

Create Quantitation Set - Create Default Query
Please specify the concentrations/sample names and the corresponding allowed accuracy variations (in percent). You can leave any of the "variation" fields empty as desired.
Maximum Allowed Accuracy Variation for QCs (%)
Concentration
Max. Variation
Maximum Allowed Accuracy Variation for Standards (%)
Concentration
Max. Variation
Query By Name
< Back
Next >
Finish
Cancel
Help

7. In the **Maximum Allowed Accuracy Variation for QCs (%)** table in the **Max. Variation** column, type the maximum allowable percent of variation for each QC (for example, 5 is ± 5%) in the same row as the corresponding concentration. If the concentrations were not specified during acquisition, they are not shown here. In that case, type them in the **Concentration** column.
8. In the **Maximum Allowed Accuracy Variation for Standards (%)** table, in the **Max. Variation** column, type the maximum allowable percent of variation for each

standard (for example, 10 is ±10%) in the same row as the corresponding concentration. If the concentrations were not specified during acquisition, they are not shown here. In that case, type them in the **Concentration** column.

9. Click **Next**.

Figure 11-3 Create Quantitation Set - Select Method Page


Create Quantitation Set - Select Method
Specify which method will be used for this quantitation set, or create a new method now.
Integration Algorithm: Analyst Classic
Choose Existing Method
Method: New Method 2.qmf
Create New Method
Method Name:
Create "Automatic" Method (to tabulate area for each available ion)
< Back
Next >
Finish
Cancel
Help

10. Select or create a method.
11. Click **Finish**.

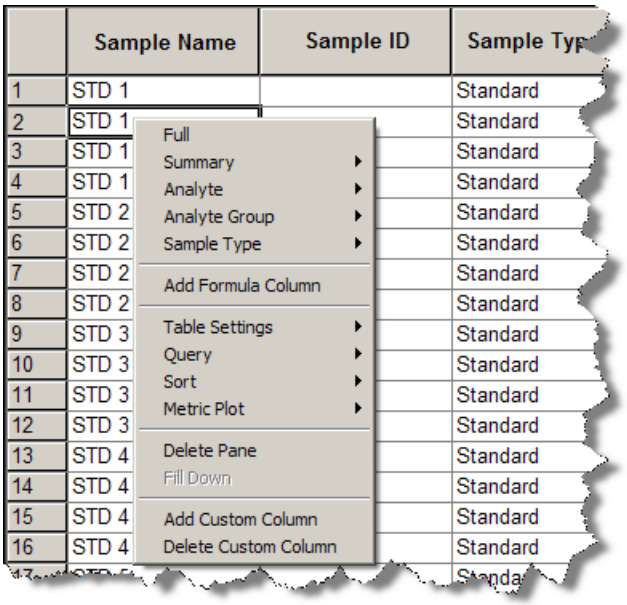
    The query is applied as a standard query. The query results are shown as a **Pass** or **Fail** entry in the **Standard Query Status** column of the Results Table.

Tip! To return to the full view, right-click and then click **Full**.

Results Table Right-Click Menu

Right-click in the Results Table table to access the following options.

Figure 11-4 Results Table Right-Click Menu



Menu	Function
Full	Shows all the columns.
Summary	Shows specific columns.
Analyte	Shows a specific analyte.
Analyte Group	Creates an analyte group.
Sample Type	Shows samples of a specific type or all samples.
Add Formula Column	Adds a formula column. It is recommended that the user validate the results if a formula column is used.
Table Settings	Edits or selects a table setting.
Query	Creates or selects a query.
Sort	Creates a sort or sorts by index.
Metric Plot	Creates a metric plot.
Delete Pane	Deletes the active pane.
Fill Down	Fills the same data into the selected cells.
Add Custom Column	Adds a custom column.
Delete Custom Column	Deletes the selected custom column.

Peak Review and Manual Integration of Peaks

Use peak review to survey the peaks that the software has identified, and then redefine the peak or the start and end points where necessary.

After identifying the analytes and internal standards that the software must find, the software searches for the peaks in the samples. When the software identifies a peak, it shows the chromatograms for each analyte and internal standard in the **Create Quantitation Method: Define Integration** page of the **Standard Wizard** or on the **Integration** tab of the **Full Method Editor**. The user can confirm the peaks that are found or change the quantitation method to better define the peaks.

Review Peaks

During peak review, the user may want to view a peak in its entirety—or may want to examine the baseline to find out how well the software found the start and end points of the peak. Use the automatic zooming feature to do either.

To help the software find a peak, define the exact start and end points of the peak and background manually. These changes will apply only to that individual peak unless the global method is updated.

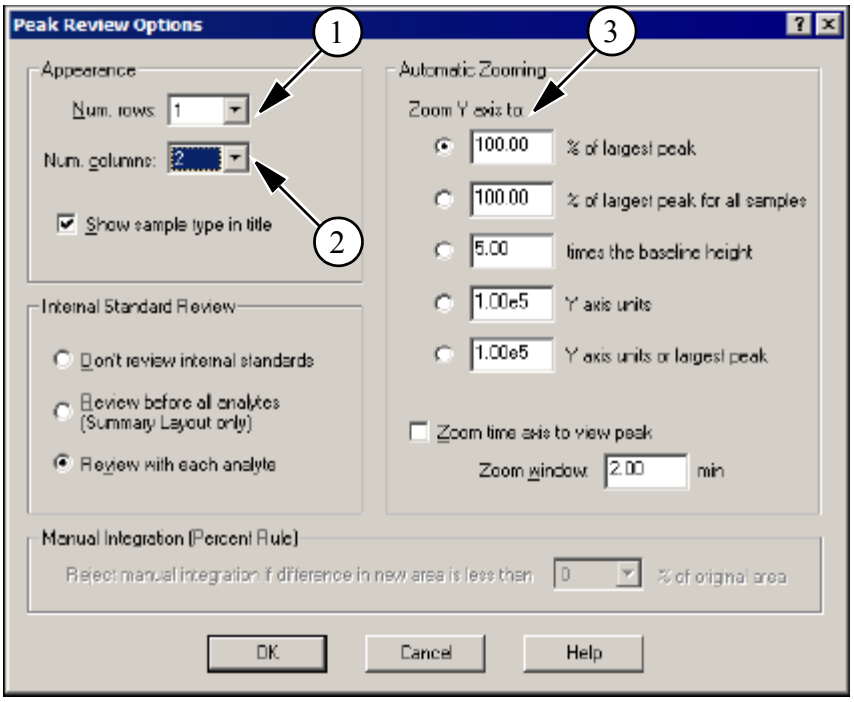
Note: It is recommended that the user validate manually integrated results.

Tip! To review an individual peak, right-click on a point on the curve and then click **Show Peak**. The software shows the **Peak Review** window with the selected peak.

1. Right-click in the **Results Table**, click **Analyte**.
2. Select a sample.
3. Click **Tools > Peak Review > Pane**.

   The peaks are shown below the Results Table with only the peaks listed in the Results Table.
4. Right-click in the pane and then click **Options**.
5. In the **Peak Review Options** dialog, in the **Appearance** section, change **Num. rows** to **1** and **Num. columns** to **2**.
6. In the **Automatic Zooming** section, click **Zoom Y axis to**: **100% of largest peak** to show the entire peak.

Figure 11-5 Peak Review Options Dialog


Peak Review Options
1
2
3
Appearance
Num. rows: 1
Num. columns: 2
Show sample type in title
Automatic Zooming
Zoom Y axis to:
100.00 % of largest peak
100.00 % of largest peak for all samples
5.00 times the baseline height
1.00e5 Y axis units
1.00e5 Y axis units or largest peak
Zoom time axis to view peak
Zoom window: 2.00 min
Internal Standard Review
Don't review internal standards
Review before all analytes (Summary Layout only)
Review with each analyte
Manual Integration (Percent Rule)
Reject manual integration if difference in new area is less than 0 % of original area
OK
Cancel
Help

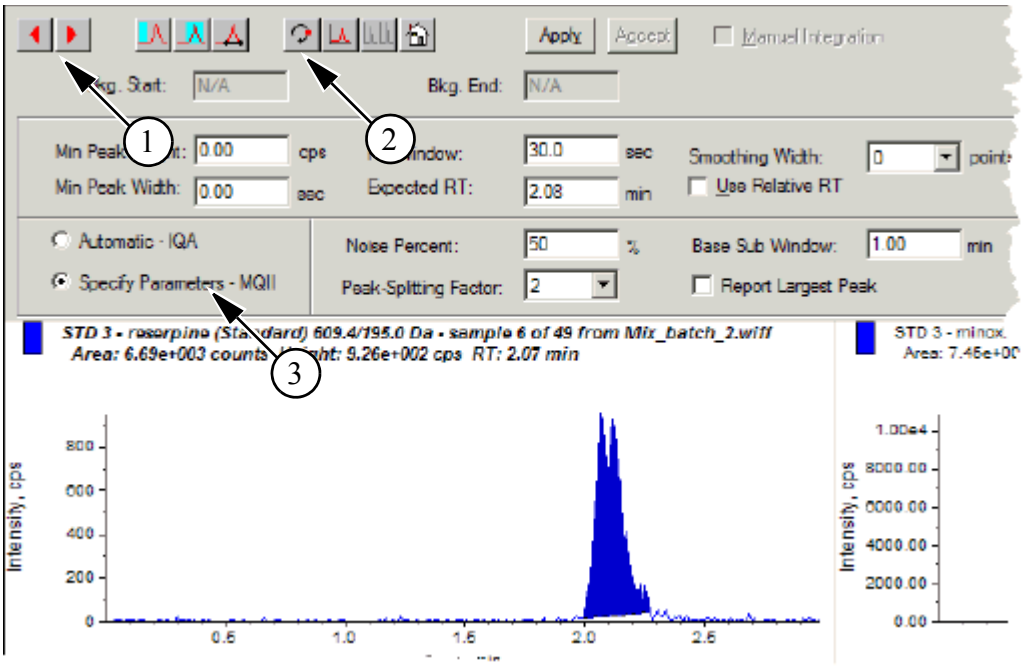
Item	Definition
1	Number of rows
2	Number of columns
3	**Zoom Y-axis to** 100**% of largest peak** to show the entire peak

7. Click **OK**.
8. To move through the peaks, click the right-pointing arrow. Refer to Figure 11-6.
9. Go to the second injection of standard 3.

   In this example, the peak can be integrated closer to the baseline by selecting the **Specify Parameters** option.

Tip! To move to a specific peak in the **Peak Review** pane, select the corresponding row in the Results Table.

Figure 11-6 Peak Review Pane



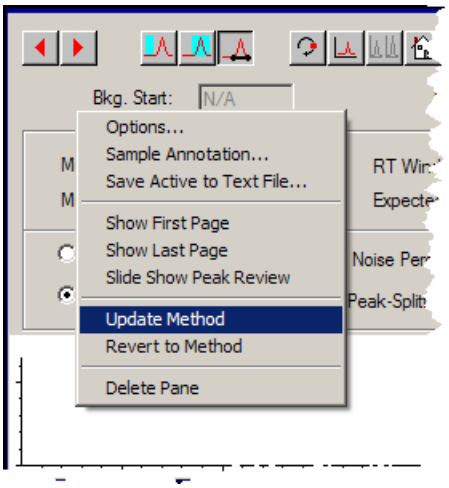
Item	Description
1	Arrows: Click to move through the peaks.
2	Show or Hide Parameters: Click to show the integration parameters.
3	Integration parameters: Click to change the parameters.

10. Click **Show or Hide Parameters** twice.
11. Click **Specify Parameters - MQ III**.
12. Change the **Noise Percent** value.
13. Click **Apply**.

    The peak is integrated closer to the baseline.
14. If the change does not improve the peak integration, then adjust the **Noise Percent** parameter until the optimal value is found.
15. To update the algorithm for all peaks, right-click in the pane and then click **Update Method**.

Note: The **Update Method** function only updates the algorithm values for that specific analyte (or internal standard) and not all analytes.

Figure 11-7 Update Method



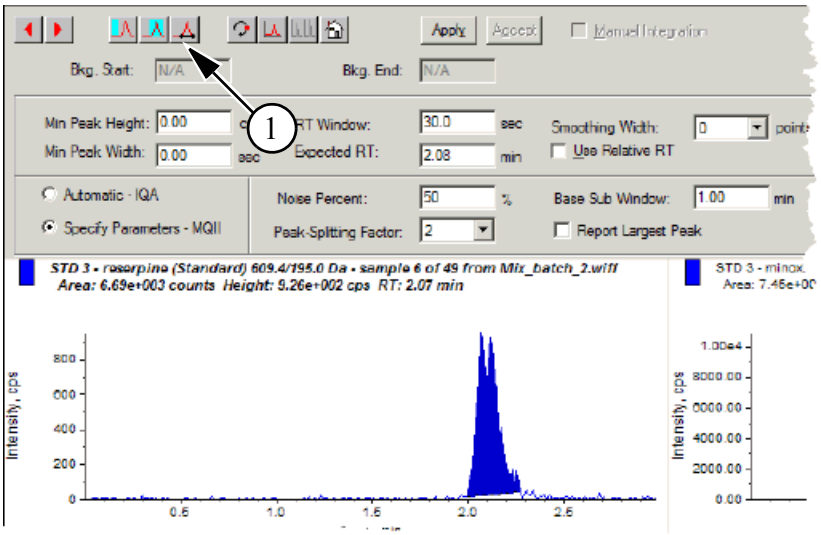
Manually Integrate Peaks

Manually integrating peaks should be done last, to limit person-to-person variability. Manually integrate peaks only if all the peaks have not been found after the algorithm parameters have been adjusted and updated.

Note: Peaks that are manually integrated, or where the algorithm was changed for only that peak, are identified as such in the **Record Modified** column of the Results Table, as are peaks that have algorithm parameter changes for a sample that are not applied to the entire analyte group.

1. In the **Peak Review** pane, click **Manual Integration Mode**.

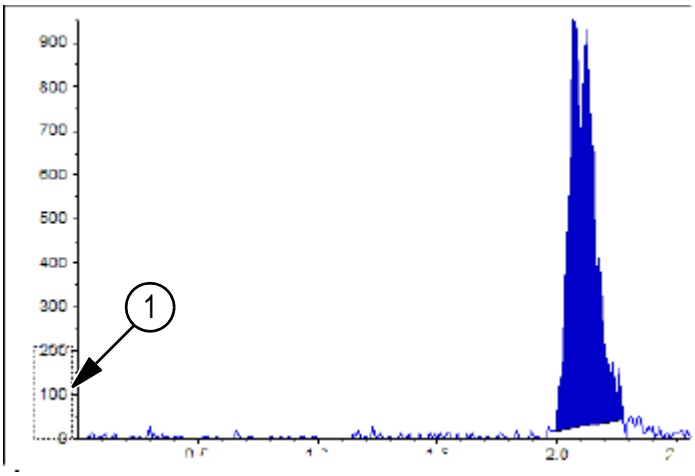
Figure 11-8 Peak Review Pane: Manual Integration



Item	Description
1	Manual Integration mode

2. Zoom in on the lower 10% of the peak.

Figure 11-9 Peak Review Pane: Zooming in on a Peak



Item	Description
1	Lower 10% of the peak

3. Position the cross-hair where the start of the peak is to be defined and then drag the cross-hair to where the end of the peak is to be defined.

   The software shades the area bounded by the base and sides of the peak. Peak parameters are gray as they are no longer applicable because the peak was drawn manually.

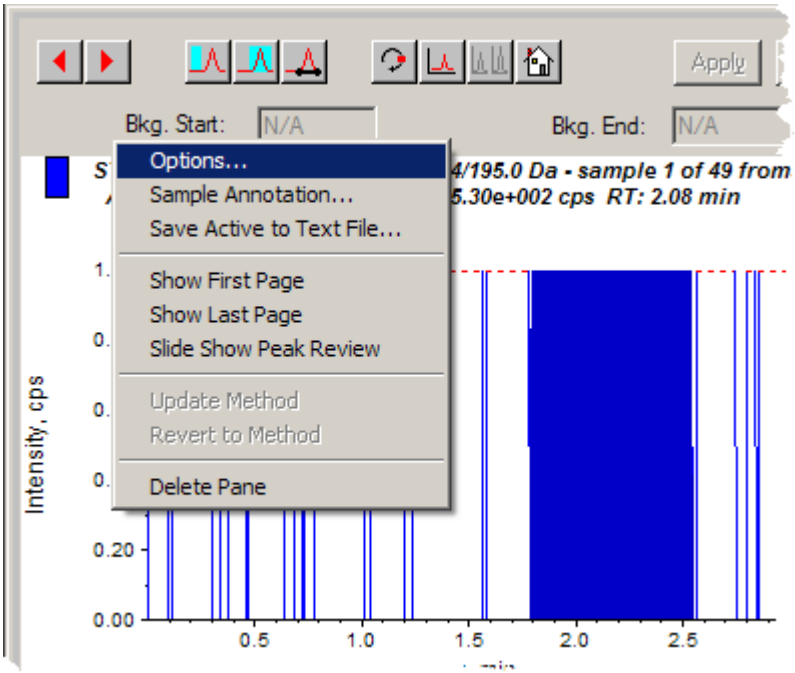
4. Do one of the following:
   - To make this change permanent, click **Accept**.
   - To discard the changes, clear the **Manual Integration** check box.

Tip! If a peak was correct as originally selected, right-click the peak and then click **Revert to Method**.

Peak Review Right-Click Menu

Right-click in the **Peak Review** window or pane to access the following options.

Figure 11-10 Peak Review Right-Click Menu



Menu	Function
Options	Opens the **Peak Review Options** dialog.
Sample Annotation	Opens the **Sample Annotation** dialog.
Save Active to Text File	Saves the selected peak as a text file.
Show First Page	Goes to the first sample.
Show Last Page	Goes to the last sample.
Slide Show Peak Review	Opens the slide show.
Update Method	Updates the algorithm for all peaks.
Revert to Method	Selects a redefined peak based on the current quantitation method.
Delete Pane	Deletes the active pane.

Calibration Curves

Use calibration curves to find the calculated concentration of samples, including quality control (QC) samples. QC samples are added to a batch to estimate the data quality and accuracy of standards in the batch. QC samples have known analyte concentrations but are treated as unknowns so that the measured concentrations can be compared to the actual value.

The calibration curve is generated by plotting the concentration of the standard versus its area or height. If an internal standard is used, the ratio of the standard concentration/internal standard

versus the ratio of the standard peak height or area to the internal standard peak height or area is plotted. The area or height ratio of a sample is then applied to this curve to find the concentration of the sample, as shown in the Results Table. A regression equation is generated by this calibration curve according to the regression that was specified. The regression equation is used to calculate the concentration of the unknown samples.

View Calibration Curves

The user can view the calibration curve and change the regression options in an open Results Table. If two or more Results Tables are open, the calibration curves can be overlaid. To overlay curves, the method used to create the tables must be the same.

Plot a calibration curve to see the curve used for regression. The **Calculated Concentration** field in the Results Table reflects any changes resulting from the fit of the curve to the points of the standard.

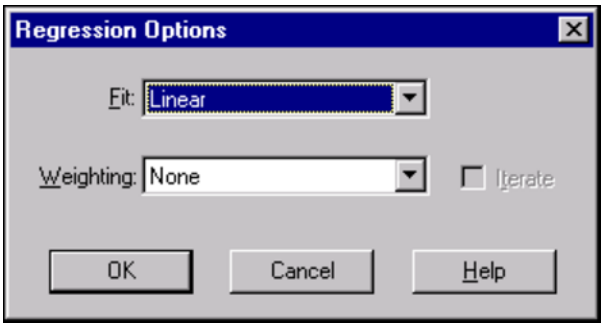
Note: This option is available only when a Results Table is open in the workspace.

1. With a Results Table open, click **Tools > Calibration > Pane**.

   The Calibration Curve pane containing the calibration curve opens.

2. If there is more than one analyte, then use the following steps to view the calibration curve for another analyte:
   i. In the **Analyte** list, select an analyte.
   ii. If required, in the next list, select **Area** or **Height**.
3. To change the regression options for the calibration curve, do the following:
   i. Click **Regression**.

Figure 11-11 Regression Options Dialog



   ii. In the **Fit** list, select **Linear**.
   iii. In the **Weight** list, select **1 / x**.
   iv. Click **OK**.

   The calibration curve opens. The user can review individual peaks on the curve or exclude points from the curve to produce a better curve.

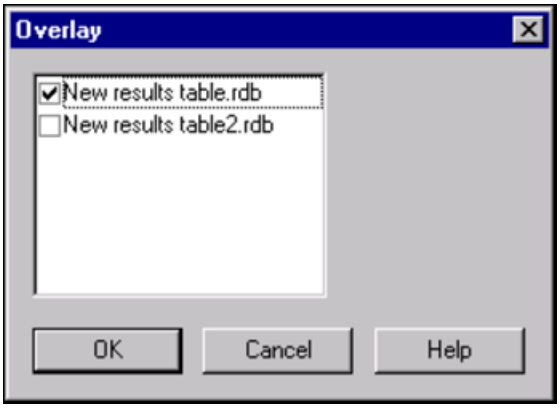
4. If required, repeat these steps to create a more appropriate curve.
5. To save the changes, click **Accept**.

Overlay Calibration Curves

Note: To examine the curve for one table more closely, right-click the curve and click **Active Plot**. Select the curve to be plotted on top.

1. With two or more open Results Tables, view a calibration curve for one of the tables.
2. Right-click the calibration curve and then click **Overlay**.

Figure 11-12 Overlay Dialog



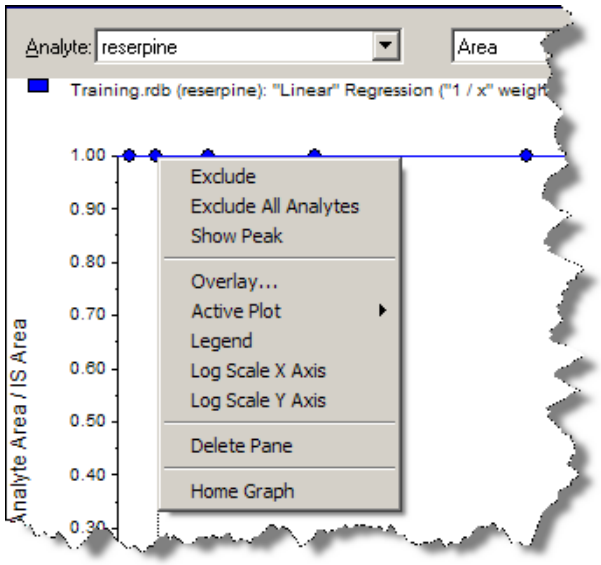
3. Select the tables to overlay with the current curve.
4. Click **OK**.

   The software plots the curves for all selected tables on the same graph.

Calibration Curve Right-Click Menu

Right-click in the Calibration window or pane table to access the following options.

Figure 11-13 Calibration Curve Right-Click Menu



Menu	Function
Exclude (Include)	Right-click the point and then click **Exclude** to exclude the point from the curve. Right-click the point and then click **Include** to include the dropped point.
Exclude All Analytes (Include All Analytes)	Right-click a point and then click **Exclude All Analytes** to exclude all the analytes from the curve. Right-click a point and then click **Include All Analytes** to include the points.
Show Peak	Reviews an individual peak.
Overlay	Overlays two graphs.
Active Plot	Determines which plot is active.
Legend	Shows the graph legend.
Log Scale X Axis*	Uses a log scale for the x-axis.
Log Scale Y Axis*	Uses a log scale for the y-axis.
Delete Pane	Deletes the active pane.
Home Graph	Scales the graph to its original size
* A log scale arranges the data points in a more manageable view so that the effect of all points can be monitored simultaneously. For this view, select Log Scale Y Axis versus Log Scale X and not just the log of one axis.	

Sample Statistics

Use the **Statistics** window to view the statistics samples, typically for standards and QCs (quality controls). The data from each available batch in the Results Table opens in tabular form in the grid and a row of data is shown for each standard or QC concentration.

View the Statistics for Standards and QCs

When viewing more than one Results Table, statistical information about the standards and QCs for additional batches in the Statistics window can be obtained. This allows the user to compare results between batches and look for trends in the standards or QCs.

1. With a Results Table open, click **Tools > Statistics**.
2. In the **Statistics Metric** list, select **Concentration**.
3. In the **Analyte Name** field, select an analyte.
4. In the **Sample Type** field, select **Standard**.

   The results are shown.
5. Look at the **%CV** and **Accuracy** columns.

   The %CV shows the coefficient of variance between the measurements of a single parameter, for example the area. Accuracy shows how close the plotted point is to the interpolated value.

6. If required, select the **Display Low/High values** check box and then examine the **Low**, **High**, and **Mean** for each row in the grid. Each row represents standards that have the same concentration levels.
7. Select another analyte.

   The results are shown on a per-analyte basis.
8. To check for Quality Control variations at the same concentration levels, select **QC** in the **Sample Type** field.

Compare Results Between Batches

The number of analytes and the analyte names must be the same for the data to be combined in the Statistics pane.

1. Open the Results Tables.
2. Click **Tools > Statistics**.
3. Do one of the following:
   - To arrange the results by Results Table, in the **Conc. as Rows** list, select **Group By Batch**.
   - To arrange the results in order of concentration, in the **Conc. as Rows** list, select **Group By Concentration**.
   - To arrange the results in order of concentration, but without a row showing the statistics for each group or batch, in the **Conc. as Rows** list, select **Group By Concentration (no All)**.

   The software sorts the results. At the end of each batch or group, one or two additional rows are shown: **All** (statistics for all results tables in that group) and **Average** (statistics on the statistics for that batch or group).

Table 11-1 Integration Tab and Quantitation Wizard Icons

Icon	Name	Function
	Set parameters from Background Region	Uses the selected peak.
	Select Peak	Uses the selected background.
	Manual Integration Mode	Manually integrates peaks.
	Show or Hide Parameters	Toggles the peak-finding parameters between shown and hidden.
	Show Active Graph	Shows the analyte chromatogram only.
	Show Both Analyte and IS	Shows the analyte and its associated chromatogram (available only when an associated internal standard exists).

Table 11-1 Integration Tab and Quantitation Wizard Icons (Continued)

Icon	Name	Function
	Use Default View for Graph	Returns to the preset (view all data) view (if, for example, the user has zoomed in on a chromatogram).

Table 11-2 Results Table Icons

Icon	Name	Function
	Sort Ascending by Selection	Sorts the selected column by ascending values.
	Sort Descending by Selection	Sorts the selected column by descending values.
	Lock or Unlock Column	Locks or unlocks the selected column. A locked column cannot be moved.
	Metric Plot by Selection	Creates a metric plot from the selected column.
	Show all Samples	Shows all the samples in the Results Table.
	Delete Formula Column	Deletes formula columns.

Table 11-3 Icon Quick Reference: Quantitate Mode

Icon	Name	Function
	Add/Remove Samples	Adds or removes samples from the Results Table.
	Export as Text	Saves the Results Table as a text file.
	Modify Method	Opens a .wiff file.
	Peak Review - Pane	Opens peaks in a pane.
	Peak Review - Window	Opens peaks in a window.
	Calibration - Pane	Opens the calibration curve in a pane.
	Calibration - Window	Opens the calibration curve in a window.

Table 11-3 Icon Quick Reference: Quantitate Mode (Continued)

Icon	Name	Function
	Show First Peak	Shows the first peak in the pane or window.
	Show Last Peak	Shows the last peak in the pane or window.
	Show Audit Trail	Shows the audit trail for the Results Table.
	Clear Audit Trail	Clears the audit trail for the Results Table.
	Statistics	Opens the **Statistics** window.
	Report Generator	Opens the **Reporter** software.

Reporter Software 12

The Reporter software extends the reporting functionality available in the Analyst® software.

It is recommended that the user validate the results if a Reporter template that contains a query is used.

Overview

The Reporter software can be used to create custom reports with Microsoft Word and Excel (2007, 2010, or 2013). The Reporter software has the following features:

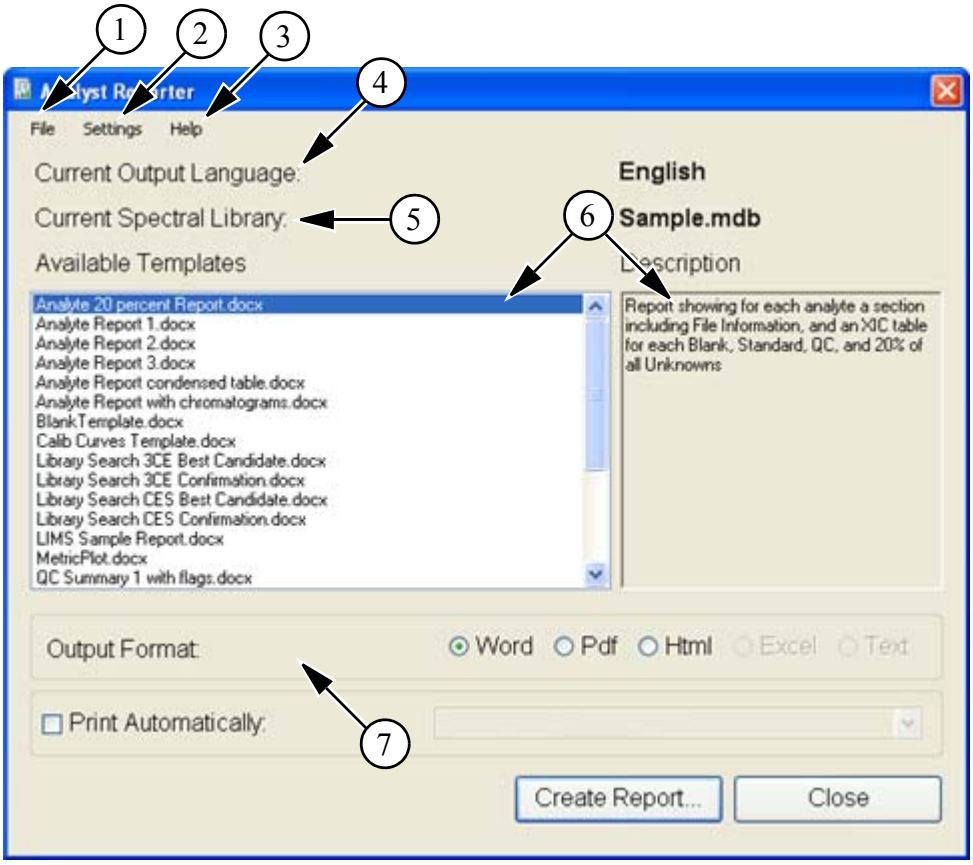
- Provides a variety of reports that use the data available in a Results Table, in file information, and in quantitative peak review windows.
- Uses Microsoft Word templates to provide the format information needed when generating reports. These templates can be created or modified to provide customized report formats. Refer to the Help if you want to create or edit templates using the Report Template Editor.
- Contains a blank starting template that can be used in the Analyst software Reporter editing environment to design report templates to meet most report requirement.
- Automates report generation through the use of the Autoquan Reporter batch script.
- Automatically prints, exports to Adobe Portable Document Format (pdf), and delivers results by e-mail. This functionality requires the Save as PDF (Office 2007) addin that is installed by the Analyst software.
- Attaches processing scripts to report templates to expand both the content and automation level for various workflow requirements.
- Generates reports from custom software applications that use the available Analyst software programming libraries.

Reporter software can be used in three ways:

- Within the Analyst software to manually generate a report or set of reports.
- By a batch script to automate report generation within a batch. You can generate reports on a sample-by-sample basis, either during or after batch acquisition.
- By applications that do not use the Analyst software.

Reporter User Interface

Figure 12-1 User Interface



Item	Option	Description
1	File > Exit	Exits the program and releases all resources.
2	Settings > Select Output Language	Sets the language dictionary that will be used to replace language tags within a report template. Templates that contain language tags within them can be used to generate reports in any language. The language tags are replaced with text from a matching tag in the dictionary file for the selected language. These dictionary files are contained in the folder: C:\Program Files\AB SCIEX\AnalystReporter\Resources \Languages.
2	Settings > Select Library	Browse to an spectral library. This library will be used for matching and scoring MS/MS from Results Tables that contain data from information dependent acquisition (IDA) triggered MS/MS.
2	Settings > Select Template Folder	Sets the folder from which the available templates will be read. To return to the default template folder, select the **Default** option.
3	Help > About	Shows information about the version of Reporter software currently installed.

Item	Option	Description
4	Current Output Language	Displays the currently selected language dictionary used for replacing language tags within a report template. The language dictionary can be selected using **Settings > Select Output Language**.
5	Current Spectral Library	Displays the currently selected spectral library. The spectral library can be selected using **Settings > Select Library**.
6	Available Templates and Description	Displays a list of available report templates. Selecting a template will show a description of the template. To change the folder where available templates are read from, select **Settings > Select Template Folder > Browse**.
7	Output Format	The Reporter software supports several output formats. Only formats that are compatible with the selected report template are enabled. • Word: Microsoft Word document (.docx) is produced. This document can be viewed by Microsoft Word 2007 and above. • PDF: The PDF option creates a report directly in PDF format. • HTML: Microsoft Word is used to generate an HTML file. Associated image files are stored in a folder with the same name as the HTML file. • Excel: A plain text file (.csv) is produced. Report templates that contain values separated by commas can be opened in Microsoft Excel, where each value will be displayed in a separate cell. Only templates that are specifically marked as text-compatible can be used for this output format. • Text: A plain text document (.txt) is produced. Only templates that have been specifically marked as text-compatible can be used for this output format. • Print Automatically: If selected, after the report has been created it is printed to the selected printer. Select from any available printer.

Generate Reports

The Reporter software extracts numerical data from the Results Table and sample and graphical information from the .wiff file.

You can select a template in the Available Template field.

Tip! For reports that can be generated on a sample-by-sample basis, it may be more efficient to generate the reports automatically using a batch script during acquisition to avoid long processing times at the end of the acquisition. For more information about batch scripts, refer to the *Scripts User Guide*.

1. Open a Results Table.
2. Under **Companion Software**, double-click **Reporter 3.2**.
3. In the Analyst Reporter dialog, in the **Available Templates** field, select a template.
4. Click an output format.

   The Word option is pre-selected and the report is automatically saved in the current project Results folder. If this option is not selected, then the report is created and opened in Word or printed as selected, but the report is not saved. This lets you edit the report in Word prior to saving the original report.
5. Select either one document containing all samples or multiple documents with one sample in each.
6. Select the **Print Automatically** check box if you want your reports to print automatically to a pre-selected printer.

   The Default Printer set in Windows is used unless you select a different printer. The Reporter tool retains the selected printer between operations. If the printer is set to a .pdf printer driver, then you can use the Analyst Reporter to generate .pdf file versions of the created reports automatically.
7. Click **Create Report**.

   The screen shows various progress indicators as the tool opens the template and populates it with data from the Results Table. Some reports may take seconds to generate, others may take longer. A large data set with many MRM transitions or a large number of graphics could result in reports of several hundred pages and could take hours to generate.

Table 12-1 Icons in Quantitate Mode

Icon	Name	Function
	Report Generator	Click to open the Reporter software.

Regularly clean and maintain the system for optimal performance. For information on tuning frequency, refer to Table B-1. For information on maintaining the ion source, refer to the ion source *Operator Guide*.

WARNING! Potential Radiation Hazard, Biohazard, or Toxic Chemical Hazard: Determine whether instrument decontamination is required prior to cleaning. Decontamination should be conducted prior to cleaning if radioactive materials, biological agents, or toxic chemicals have been used with an instrument.

Table 13-1 provides a recommended schedule for cleaning and maintaining the system. Contact a Qualified Maintenance Person (QMP) to order consumable parts. Contact an AB SCIEX representative for maintenance service and support.

Table 13-1 Maintenance Tasks

Component	Frequency	Task	For more information...
Curtain plate	Daily	Clean	Refer to Clean the Curtain Plate on page 126.
Orifice plate (front)	Daily	Clean	Refer to Clean the Front of the Orifice Plate on page 126.
Orifice plate (front and rear)	As needed	Clean	Contact the local QMP or AB SCIEX Field Service Employee (FSE).
IonDrive QJet® ion guide	As needed	Clean	Contact the local QMP or FSE.
Q0 and IQ1 lens	As needed	Clean	Contact the local QMP or FSE.
Instrument surfaces	As needed	Clean	Refer to Clean the Surfaces on page 122
Drain bottle	As needed	Empty	Refer to Empty the Source Exhaust Drain Bottle on page 127
Roughing pump oil	As needed	Check and fill	Contact the local QMP or FSE.
Instrument air filter	Every 6 months	Inspect and clean or replace	Contact the local QMP or FSE.
Roughing pump oil	Annually	Replace	Contact the local QMP or FSE.
Electrode	As needed	Inspect and clean or replace	Refer to the *IonDrive™ Turbo V Ion Source Operator Guide*.
Corona discharge needle	As needed	Replace	Refer to the *IonDrive™ Turbo V Ion Source Operator Guide*.

For “As needed” tasks, follow these guidelines:

- Clean the QJet ion guide and Q0 region if system sensitivity degrades.

Tip! Clean the Q0 region regularly to minimize the impact of charging (a significant loss of sensitivity of the ions of interest over a short period of time) on the quadrupoles and lenses. Contact a Qualified Maintenance Person or AB SCIEX Field Service Employee (FSE).

- Clean the mass spectrometer surfaces after a spill, or when they become dirty.
- Empty the drain bottle before it becomes full.

Clean the Surfaces

Clean the external surfaces of the mass spectrometer after a spill or when they become dirty.

1. Wipe the external surfaces with a soft cloth dampened with warm, soapy water.
2. Wipe the external surfaces with a soft cloth moistened with water to remove any soap residue.

Clean the Front-End

Clean the mass spectrometer front-end using the routine cleaning method, to:

- Minimize unscheduled system downtime.
- Maintain optimum sensitivity.
- Avoid more extensive cleaning that requires a service visit.

Symptoms of contamination: Significant loss in sensitivity and increased background noise.

When contamination occurs, perform an initial routine cleaning. Clean up to and including the front of the orifice plate. If routine cleaning does not resolve issues with sensitivity, a full cleaning may be necessary.

This section provides instructions for performing routine cleaning without breaking vacuum and full cleaning under atmospheric pressure, after venting the mass spectrometer.

Note: Follow all applicable local regulations. For health and safety guidelines, refer to Chemical Precautions on page 11.

Note: U.S. customers can call 877-740-2129 for ordering information and inquiries. International customers can visit www.absciex.com.

Required Materials

• Powder free gloves (nitrile recommended)
• Safety glasses
• Laboratory coat
• Fresh, high quality water (at least 18 Mohm de-ionized water (DI) or ultra-pure HPLC-grade water). Old water can contain contaminants which can further contaminate the mass spectrometer.
• HPLC- or MS-grade methanol, isopropanol (2-propanol), or acetonitrile
• Cleaning solution. Use one of:
  • 100% methanol
  • 100% isopropanol
  • 50:50 acetonitrile:water solution (freshly prepared)
  • 50:50 acetonitrile:water with 0.1% acetic acid solution (freshly prepared)

Table 13-2 Tools and Supplies Available from AB SCIEX

Description	PN
Small polyester swab (thermally bonded). Available in the Cleaning kit.	5021294
Small lint-free wipe (11 cm x 21 cm). Available in the Cleaning kit.	018027

Best Practices

WARNING! Toxic Chemical Hazard: Follow all safety guidelines and applicable local regulations when handling, storing, and disposing of chemicals. For health and safety guidelines, refer to Chemical Precautions on page 11**.**

WARNING! Potential Radiation Hazard, Biohazard, or Toxic Chemical Hazard: Determine whether decontamination is required prior to cleaning. Decontamination should be conducted prior to cleaning if radioactive materials, biological agents, or toxic chemicals have been used with the system.

WARNING! Environmental Hazard: Do not dispose of system components, cleaning materials, or chemicals in municipal waste. Follow established procedures when disposing of components, cleaning materials, and chemicals.

- Always wear clean, powder-free gloves for the cleaning procedures.
- After cleaning the mass spectrometer components and before reassembling them, put on a clean pair of gloves.
- Do not use cleaning supplies other than those specified in this procedure.
- Prepare cleaning solutions just before beginning the procedure, if possible.
- Prepare and store all organic solutions and organic-containing solutions in very clean glassware only. Never use plastic squirt bottles. Contaminants can leach from these bottles and further contaminate the mass spectrometer.
- Allow only the center area of the wipe to contact the instrument surface. Cut edges can leave fibers behind.

Tip! Wrap the wipe around a thermally-bonded polyester swab.

Figure 13-1 Example: Folding the Wipe

- To avoid cross-contamination, allow the wipe or swab to contact the surface once, and then discard it.
- Larger parts of the vacuum interface, such as the curtain plate, may require several cleanings, using multiple wipes.
- To avoid contaminating the solution, pour the solution on the wipe or swab.

- Only dampen the wipe or swab slightly when applying water or cleaning solution. Water, more so than organic solvents, may cause the wipe to deteriorate, leaving residue on the mass spectrometer.

Prepare for Cleaning

In routine cleaning, clean the curtain plate and the front of the orifice plate. Routine cleaning can be performed while the mass spectrometer remains under vacuum.

Note: Mass spectrometers with a NanoSpray® ion source may require a full cleaning for best results. Contact an FSE.

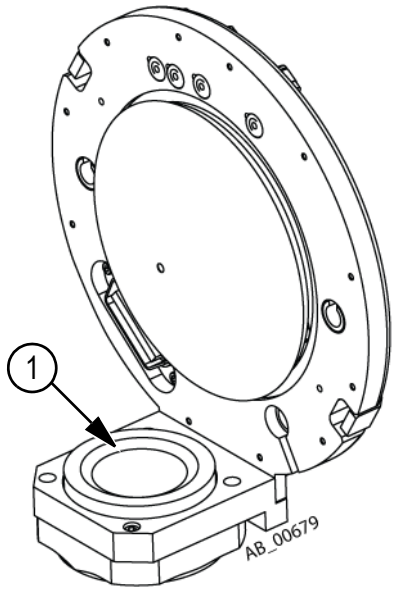
1. Deactivate the hardware profile.

WARNING! Hot Surface Hazard: Surfaces of the IonDrive™ Turbo V ion source become hot during operation. Let the ion source and vacuum interface components cool for at least 90 minutes before starting any cleaning procedures.

2. Wait at least 90 minutes for the ion source, curtain plate and orifice plate to cool.
3. Remove the ion source. Be sure to place the ion source in a safe location.

Caution: Potential System Damage. Be careful not to not drop anything into the source drain when the ion source is removed.

Figure 13-2 Source Drain on the Vacuum Interface



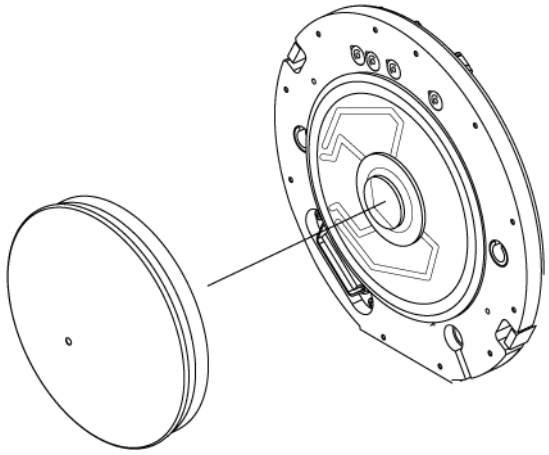
Item	Description
1	Source drain

Clean the Curtain Plate

Caution: Potential System Damage: Do not rest the curtain plate on the aperture tip. Make sure that the conical side faces up.

1. Remove the curtain plate and put it, conical side up, on a clean, stable surface.

Figure 13-3 Interface with Curtain Plate Removed



2. Dampen a lint-free wipe with water and clean both sides of the curtain plate. Use multiple wipes, as required.
3. Repeat step 2 using the cleaning solution.
4. Using a dampened wipe or small poly swab, clean the aperture.
5. Wait until the curtain plate is dry.
6. Inspect the curtain plate for solvent stains or lint, removing any residue with a clean, slightly damp lint-free wipe.

Note: Persistent spotting or filming is an indicator of contaminated solvent.

Clean the Front of the Orifice Plate

Tip! Use the correct orifice plate for the system. Do not use an orifice plate for another system. The model number for the system is etched into the orifice plate.

Note: If you are cleaning the standard orifice plate and it has a removable interface heater, do not remove the heater.

1. When cleaning a NanoSpray orifice plate, remove the interface heater and clean it:
   i. Wipe the heater with a lint-free wipe dampened with water.
   ii. Wipe the heater with a lint-free wipe dampened with cleaning solution.

2. Dampen the lint-free wipe with water and then wipe the front of the orifice plate.

Caution: Potential System Damage: Do not insert a wire or metal brush into the aperture, to avoid damaging the aperture.

3. Repeat step 2 using the cleaning solution.
4. Wait until the orifice plate is dry.
5. Inspect the orifice plate for solvent stains or lint, removing any residue with a clean, slightly damp lint-free wipe.

Note: Persistent spotting or filming is an indicator of contaminated solvent.

Put the System Back into Service

1. Install the curtain plate on the front end of the mass spectrometer.
2. Install the ion source on the mass spectrometer. Refer to the ion source *Operator Guide*.
3. Activate the hardware profile.

Empty the Source Exhaust Drain Bottle

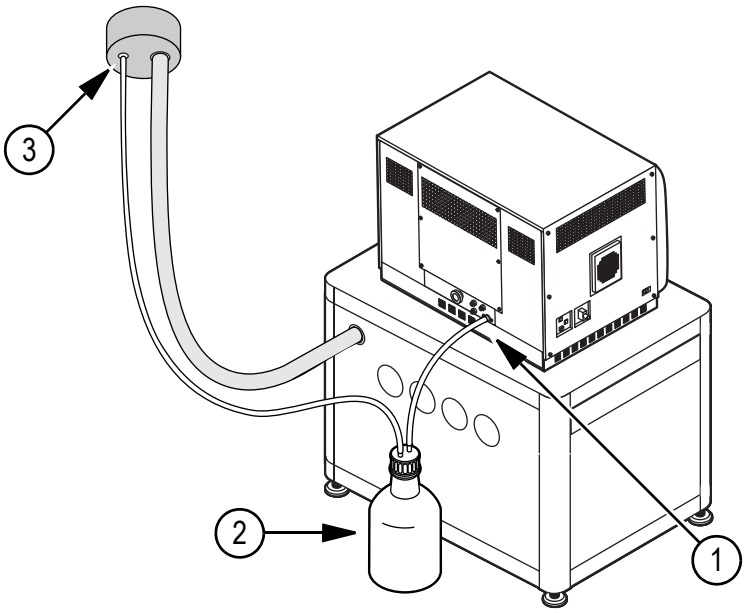
Empty the source exhaust drain bottle before it becomes full.

WARNING! Radiation Hazard, Biohazard, or Toxic Chemical Hazard: Deposit hazardous material in appropriately labelled containers. Potential risk of personal injury if proper procedures for handling and disposing of hazardous materials are not followed.

WARNING! Hot Surface Hazard: Surfaces of the IonDrive™ Turbo V ion source become hot during operation. Let the ion source and vacuum interface components cool for at least 90 minutes before starting any cleaning procedures.

1. Remove the ion source. Refer to the ion source *Operator Guide*.
2. Loosen the clamps connecting the hoses to the cap of the source exhaust drain bottle.
3. Remove the drain bottle from the cap.

Figure 13-4 Source Exhaust Drain Bottle



Item	Description
1	Connection to mass spectrometer
2	Source exhaust drain bottle
3	Connection to vent **Caution: Asphyxiation Hazard: Take care to vent exhaust gases properly. The use of mass spectrometers without adequate ventilation to outside air may constitute a health hazard. In addition, certain procedures required during the operation of the mass spectrometer may cause gases to be discharged into the exhaust stream; under these conditions, inadequate ventilation may result in serious injury. Regularly perform an inspection of the hoses to make sure that there are no leaks.**

Note: Source exhaust hose connections at the drain bottle, mass spectrometer, and the lab vent are secured with a hose clamp.

4. Empty the drain bottle and then dispose of the waste.
5. Install the cap on the bottle.
6. Tighten the clamps holding the hoses to the cap.

Storage and Handling

WARNING! Environmental Hazard: Do not dispose of waste of electrical and electronic equipment as unsorted municipal waste. It must be collected separately. Contact AB SCIEX for more information concerning the decommissioning of equipment.

If the mass spectrometer needs to be stored for a long time or prepared for shipping, contact an AB SCIEX FSE for decommissioning information. To disconnect power from the mass spectrometer, remove the mains supply connector from the AC mains supply.

Note: The system must be transported and stored between -30°C to +45°C. Store the system below 2000 m above sea level.

Troubleshooting

14

This appendix contains basic information for troubleshooting basic system issues. Certain activities may be carried out by the AB SCIEX trained Qualified Maintenance Person (QMP) in the laboratory. For advanced troubleshooting, contact an FSE.

Table 14-1 System Issues

Symptom	Possible Cause	Corrective Action
Sensitivity loss	Instrument or ion source requires tuning and optimizing	For more information, refer to: • Operating Instructions — Tune and Calibrate on page 51 • Ion source *Operator Guide* • Analyst® software Help system
	Dirty curtain plate	Clean the Curtain Plate on page 126.
	Dirty orifice plate	Clean the Front of the Orifice Plate on page 126.
	Dirty IonDrive QJet® ion guide, Q0 or IQ0	Contact an FSE or the local Qualified Maintenance Person.
Frequent or extreme contamination of the QJet ion guide	Curtain Gas™ flow rate is too low.	Verify, and if applicable, increase the Curtain Gas flow rate.
Low vacuum pressure	Low roughing pump oil level.	Check the roughing pump oil level, and add oil if necessary. Contact an FSE or the local Qualified Maintenance Person.

For sales, technical assistance or service, contact an FSE or visit the AB SCIEX web site at **www.absciex.com** for contact information.

Parameters for 6500 Series Instruments

A

The following table contains generic parameters for the 6500 series of instruments. The first number under each scan type is the preset value; the range of numbers is the accessible range for each parameter.

Table A-1 Parameters for 6500 Series Instruments

Access ID	Positive ion mode			Negative ion mode		
	Q1	Q3	MS/MS	Q1	Q3	MS/MS
CUR[6]	20 10 to 55	20 10 to 55	20 10 to 55	20 10 to 55	20 10 to 55	20 10 to 55
CUR[1][2][3][4][5][7][8]	20 10 to 55	20 10 to 55	20 10 to 55	20 10 to 55	20 10 to 55	20 10 to 55
CAD[a][b]	0 Fixed	6 Fixed	Medium Low, Medium, High	0 Fixed	6 Fixed	Medium Low, Medium, High
CAD[c][d]	0 Fixed	6 Fixed	6 0 to 12	0 Fixed	6 Fixed	6 0 to 12
IS[1][2][7]	5500 0 to 5500	5500 0 to 5500	5500 0 to 5500	–4500 –4500 to 0	–4500 –4500 to 0	–4500 –4500 to 0
IS[5] Ion Transfer Voltage	1500 0 to 2500	1500 0 to 2500	1500 0 to 2500	–1500 –2500 to 0	–1500 –2500 to 0	–1500 –2500 to 0
IS[6]	1000 0 to 4000	1000 0 to 4000	1000 0 to 4000	–1000 –4000 to 0	–1000 –4000 to 0	–1000 –4000 to 0
NC[3][4][8]	3 0 to 5	3 0 to 5	3 0 to 5	–3 –5 to 0	–3 –5 to 0	–3 –5 to 0
TEM[2][3][4][5][7][8]	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750	0 0 to 750
DP	100 0 to 300	100 0 to 300	100 0 to 300	–100 –300 to 0	–100 –300 to 0	–100 –300 to 0
EP	10 2 to 15	10 2 to 15	10 2 to 15	–10 –15 to –2	–10 –15 to –2	–10 –15 to –2

(1)IonSpray™ ion source (2)TurboIonSpray® ion source (3)Heated Nebulizer (4)DuoSpray™ ion source, 1=TIS, and 2=HN (5)PhotoSpray® ion source (6) NanoSpray® ion source (7) IonDrive™ Turbo V ion source (8) Heated Nebulizer IonDrive Turbo V source (a) AB SCIEX QTRAP® 6500 system LM (Low Mass) (b) AB SCIEX QTRAP 6500 system HM (High Mass) (c) AB SCIEX Triple Quad™ 6500 system LM (d) AB SCIEX Triple Quad 6500 system HM

Table A-1 Parameters for 6500 Series Instruments (Continued)

Access ID	Positive ion mode			Negative ion mode		
	Q1	Q3	MS/MS	Q1	Q3	MS/MS
CEM	1150 0 to 3300	1150 0 to 3300	1150 0 to 3300	1150 0 to 3300	1150 0 to 3300	1150 0 to 3300
GS1	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90	20 0 to 90
GS2	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90	0 0 to 90
IHT(6)	150 0 to 250	150 0 to 250	150 0 to 250	150 0 to 250	150 0 to 250	150 0 to 250
sdp(4)	1 1 or 2	1 1 or 2	1 1 or 2	1 1 or 2	1 1 or 2	1 1 or 2
EX2	0 Fixed	0 Fixed	0 Fixed	0 Fixed	0 Fixed	0 Fixed
IQ1 (IQ1 = Q0 + offset)	Q0 + (-0.5)	Q0 + (-0.5)	Q0 + (-0.5)	Q0 + 0.5	Q0 + 0.5	Q0 + 0.5
ST1 (ST1 = Q0 + offset)	Q0 + (-10)	Q0 + (-10)	Q0 + (-10)	Q0 + 10	Q0 + 10	Q0 + 10
IE1 (IE1 = Q0 - RO1)	1.0 0 to 3	n/a	1 0 to 3	-1 -3 to 0	n/a	-1 -5 to 0
IQ2 (IQ2 = Q0 + offset)	Q0 + (-10)	Q0 + (-10)	Q0 + (-10)	Q0 + 10	Q0 + 10	Q0 + 10
RO1	n/a	Q0 + (-1)	n/a	n/a	Q0 + 1	n/a
RO2	-20 Fixed	-20 Fixed	n/a	20 Fixed	20 Fixed	n/a
CE (CE = Q0 - RO2)	n/a	n/a	30 5 to 180	n/a	n/a	-30 -180 to -5

(1)IonSpray™ ion source (2)TurboIonSpray® ion source (3)Heated Nebulizer (4)DuoSpray™ ion source, 1=TIS, and 2=HN (5)PhotoSpray® ion source (6) NanoSpray® ion source (7) IonDrive™ Turbo V ion source (8) Heated Nebulizer IonDrive Turbo V source (a) AB SCIEX QTRAP® 6500 system LM (Low Mass) (b) AB SCIEX QTRAP 6500 system HM (High Mass) (c) AB SCIEX Triple Quad™ 6500 system LM (d) AB SCIEX Triple Quad 6500 system HM

Table A-1 Parameters for 6500 Series Instruments (Continued)

Access ID	Positive ion mode			Negative ion mode		
	Q1	Q3	MS/MS	Q1	Q3	MS/MS
ST3 (ST3 = RO2 + offset)	RO2 + (-10)	n/a	n/a	RO2 + 10	n/a	n/a
CXP (CXP = RO2 - ST3)	n/a	15 0 to 55	15 0 to 55	n/a	-15 -55 to 0	-15 -55 to 0
RO3	-50 Fixed	n/a	n/a	50 Fixed	n/a	n/a
IE3	n/a	2 0 to 5	2 0 to 5	n/a	-2 -5 to 0	-2 -5 to 0

(1)IonSpray™ ion source (2)TurboIonSpray® ion source (3)Heated Nebulizer (4)DuoSpray™ ion source, 1=TIS, and 2=HN (5)PhotoSpray® ion source (6) NanoSpray® ion source (7) IonDrive™ Turbo V ion source (8) Heated Nebulizer IonDrive Turbo V source (a) AB SCIEX QTRAP® 6500 system LM (Low Mass) (b) AB SCIEX QTRAP 6500 system HM (High Mass) (c) AB SCIEX Triple Quad™ 6500 system LM (d) AB SCIEX Triple Quad 6500 system HM

Table A-2 QTRAP 6500 HM (High Mass) and LM (Low Mass) System Parameters for LIT Scan Types Only

Access ID	Positive Ion Mode	Negative Ion Mode
CUR(6)	20 10 to 55	20 10 to 55
CUR(1)(2)(3)(4)(5)(7)(8)	20 10 to 55	20 10 to 55
CAD	High Low; Medium; High	High Low; Medium; High
IS(1)(2)(7)	5500 0 to 5500	-4500 -4500 to 0
IS(5)	1500 0 to 2500	-1500 -2500 to 0
IS(6)	1000 0 to 4000	-1000 -4000 to 0
NC(3)(4)(8)	3 0 to 5	–3 –5 to 0
TEM(2)(3)(4)(5)(7)(8)	0 0 to 750	0 0 to 750

Table A-2 QTRAP 6500 HM (High Mass) and LM (Low Mass) System Parameters for LIT Scan Types Only (Continued)

Access ID	Positive Ion Mode	Negative Ion Mode
DP	100 0 to 300	–100 –300 to 0
EP	10 2 to 15	–10 –15 to –2
AF2	0.100 0 or 1	0.100 0 or 1
AF3	Mass-Speed Dependent 0 to 10	Mass-Speed Dependent 0 to 10
EXB	Mass-Speed Dependent –165 to 0	Mass-Speed Dependent 0 to 165
CEM	1150 0 to 3300	1150 0 to 3300
GS1	20 0 to 90	20 0 to 90
GS2	0 0 to 90	0 0 to 90
CES	0 0 to 50	0 0 to 50
IE1	1 0 to 5	-1 -5 to 0
CE (Q0 - ROS)	10 5 to 180	-10 -180 to -10
IHT(6)	150 0 to 250	150 0 to 250
sdp(4)	1 1 or 2	1 1 or 2

(1)IonSpray™ ion source (2)TurboIonSpray® ion source (3)Heated Nebulizer (4)DuoSpray™ ion source, 1=TIS, and 2=HN (5)PhotoSpray® ion source (6) NanoSpray® ion source (7)IonDrive™ Turbo V ion source (8) Heated Nebulizer IonDrive Turbo V source

Calibration Ions and Solutions

B

Table B-1 Tuning Frequency

	Calibration		Resolution Optimization	
Scan Type	**Frequency**	**Manual/ Automated**	**Frequency**	**Manual/Automated**
Q1 and Q3	3 to 6 months	Both	3 to 6 months	Both
LIT	Every 2 weeks; as required	Both	3 to 6 months	Automated only

Table B-2 Suggested Tuning Solutions for AB SCIEX Triple Quad™ 6500 System

System	Positive	Negative
AB SCIEX Triple Quad 6500 system (Low Mass and High Mass)	2×10^{-7} M PPG (1:500)	3×10^{-5} NEG PPG (1:10) (Neg PPG is same as PPG3000)

Table B-3 Suggested Tuning Solutions for QTRAP® 6500 LC/MS/MS System

	Q1 and Q3		LIT
Instrument	**Positive**	**Negative**	**Positive and Negative**
QTRAP 6500 LC/MS/MS system (Low Mass and High Mass)	2×10^{-7} M PPG (1:500)	3×10^{-5} NEG PPG (1:10) (Neg PPG is same as PPG3000)	1:100 Agilent mix

Table B-4 Q1 and Q3 PPG Positive Ion Scans for AB SCIEX Triple Quad 6500 System (Low Mass)

Solution	Masses						
PPG	59.05	175.133	500.38	616.464	906.673	1080.799	1196.883

Table B-5 Q1 and Q3 PPG3000 Negative Ion Scans for AB SCIEX Triple Quad 6500 System (Low Mass)

Solution	Masses			
PPG3000	44.998	585.385	933.636	1223.845

Table B-6 Q1 and Q3 PPG Positive Ion Scans for AB SCIEX Triple Quad 6500 System (High Mass)

Solution	Masses							
PPG	59.05	175.133	500.38	616.464	906.673	1254.925	1545.134	1951.427

Table B-7 Q1 and Q3 PPG3000 Negative Ion Scans for AB SCIEX Triple Quad 6500 System (High Mass)

Solution	Masses					
PPG3000	44.998	585.385	933.636	1223.845	1572.097	1862.306

Table B-8 Q1 and Q3 PPG Positive Ion Scans for QTRAP 6500 LC/MS/MS System (Low Mass)

Solution	Masses						
PPG	59.05	175.133	500.38	616.464	906.673	1080.799	1196.883

Table B-9 Q1 and Q3 PPG3000 Negative Ion Scans for QTRAP 6500 LC/MS/MS System (Low Mass)

Solution	Masses			
PPG3000	44.998	585.385	933.636	1223.845

Table B-10 Q1 and Q3 PPG Positive Ion Scans for QTRAP 6500 LC/MS/MS System (High Mass)

Solution	Masses							
PPG	59.05	175.133	500.38	616.464	906.673	1254.925	1545.134	1951.427

Table B-11 Q1 and Q3 PPG3000 Negative Ion Scans for QTRAP 6500 LC/MS/MS System (High Mass)

Solution	Masses					
PPG3000	44.998	585.385	933.636	1223.845	1572.097	1862.306

Table B-12 Masses and Polarity for the QTRAP 6500 LC/MS/MS System (Low Mass) for Agilent

Polarity	Masses			
LIT Positive	118.087	322.049	622.029	922.01
LIT Negative	112.985	431.982	601.978	—

Table B-13 Masses and Polarity for the QTRAP 6500 LC/MS/MS System (High Mass) for Agilent

Polarity	Masses				
LIT Positive	118.087	322.049	622.029	922.01	1521.972
LIT Negative	112.987	431.982	601.978	1033.988	1633.949